PROCESS DRIVEN MODELS FOR SPRAY RETENTION BY PLANTS

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Abstract

The aim of this project was to investigate and develop physical models of the process of spray retention on plants. By developing a greater understanding of the physical processes involved in spray retention it is then possible to tailor spray formulations that will be retained better on various types of plant leaves. This has great environmental and cost benefits as it is then possible to use less active chemicals to achieve the same level of uptake by the plant. Different aspects of the retention process were considered including the trajectory of the spray on leaving the nozzle; a droplet-leaf collision model allowing for bounce, shatter and retention of the droplets on the leaf surface; overall retention and runoff of spray as it accumulates on the leaf surface; and a plant canopy model to describe the interception of the spray within the plant canopy.

1. Introduction

The aim of this project was to investigate and develop physical models of the process of spray retention on plants. This depends upon many factors including the droplet distributions (size and velocity), the spray formulation's surface tension, the plants' leaf characteristics (such as being waxy or hairy), and finally the properties of the plant canopy (such as overall shape, height and the distribution of leaves and leaf angles). It is important to have good models of spray retention for the optimisation of the spraying process. For cost, and environmental

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considerations, the eventual aim should be to minimise the amount of spray agent used while ensuring that the required dose still reaches the plant. Some of the parameters of that process can be adjusted such as spray height and the formulation's surface tension while others such as the plants' leaf characteristics can not.

The MISG group divided the problem into a number of sub-problems: a spray trajectory model; a collision model; a run-off model; and a plant canopy model. From the canopy models the probability of hitting a leaf is determined. From the spray and trajectory model the droplet size and velocity is determined at the point of hitting the leaf (in fact a whole spectrum of values is required). The behaviour of the droplet and whether it bounces, adheres or shatters is determined from the collision model. Finally run-off must be monitored and allowed for. As well as their own experience and experimental results, the PPC_{NZ} representatives brought an extensive collection of papers from the scientific literature. The information therein provided a large part of the foundation for the different component models.

To construct a model of the whole retention process all of these submodels need to be brought together. Members of the MISG group constructed a flow-chart to illustrate the process and calculated retention for a simplified model by assuming some of the probabilities involved in the process.

2. Droplet Trajectory

2.1. Introduction

To be able to predict what happens to a droplet when it impacts on a leaf surface, one must know the impact conditions such as droplet size, droplet velocity, leaf angle and other leaf characteristics (such as roughness and wettability). In this section we investigate the deceleration of the droplets from the spray nozzle to the plant canopy and demonstrate a method for calculating the velocity of the droplet at impact on the leaf surface.

2.2. Velocity calculation

An individual droplet in an air stream is under the influence of three forces: the air resistance, its own weight due to gravity, and the buoyancy force due to the air displaced by the droplet. The density of the droplet is similar to that of water and hence is approximately three orders of magnitude higher than that of the surrounding air, so the buoyancy force of the droplet is very small, and can be ignored. Summing the effects

of air resistance and gravity according to Newton's second law gives the following differential equation for the velocity of the droplet

$$\begin{aligned} m\frac{d\mathbf{v}}{dt} &= -\frac{\pi}{8}C_D\rho_a d^2|\mathbf{v}-\mathbf{u}|(\mathbf{v}-\mathbf{u}) + mg\mathbf{k} \\ &= -\frac{\pi}{8}C_D\rho_a d^2|\mathbf{v}-\mathbf{u}|(\mathbf{v}-\mathbf{u}) + \frac{\pi}{6}\rho d^3 g\mathbf{k}, \end{aligned} \tag{1}$$

(cf.[18]) where $\mathbf{v}$, ρ, m and d are the velocity, density, mass and diameter of the droplet, respectively, ρ_a is the density of the surrounding air and $\mathbf{u}$ is the ambient air velocity. The drag coefficient (C_D) is dependent on the Reynolds number (Re) and is given by Perry *et al.* [18] as

$$C_D = \frac{24}{\mathrm{Re}}(1 + 0.14\mathrm{Re}^{0.70}) \qquad \text{for Re} \leq 1000, \tag{2}$$

$$C_D = 0.447 \qquad \text{for Re} > 1000. \tag{3}$$

The Reynolds number is the ratio of inertial forces to viscous forces and so here we set $Re = \rho_a|\mathbf{v}-\mathbf{u}|d/\mu_a$. We take values of $\mu_a = 1.82 \times 10^{-5}$kg/m/s for the dynamic fluid viscosity of air and $\rho_a = 1.21$kg/m^3 for the density of air.

Droplets with diameters in the range of interest (100μm - 1000μm) will mostly be in the intermediate region of flow given by equation (2). In order for equation (3) to apply, a 100μm droplet would need to have a relative speed of at least 150m/s, and a 1000μm droplet would need to have a relative speed of at least 15m/s. This latter case may occur near the point of release, as the initial speed of a droplet leaving the sprayer is typically between 15m/s and 18 m/s (from sprayer manufacturer fact sheets and personal experience of the industry representatives) and so (3) would be appropriate for a 1000μm droplet near the nozzle. However, in general, equation (2) is the applicable form of the drag coefficient.

Terminal velocity for a droplet can be obtained by solving the steady state version of equation (1) for the velocity. At terminal velocity a droplet is moving with the air horizontally, and falling toward the ground at a rate called its settling speed S, which depends on the droplet size. Some settling speeds for the range of diameters considered are given in Table 1.

In boom spraying the droplets are released from a horizontal boom which runs perpendicular to the direction of travel. As a generic example of spraying, we will consider a comparatively typical boom spraying scenario with droplets having an initial speed of 15m/s, and the boom being approximately 50cm above the crop canopy. These would be appropriate values for the spraying of short crops such as onions or potatoes. It is assumed that there is no wind. Furthermore, entrainment

Droplet Diameter (μm)	Settling Speed (m/s)
100	0.29
300	1.35
500	2.30
700	3.16
1000	4.32

Table 1. Some typical settling speeds of droplets.

of the air near the spray nozzle is not considered. These are simplifying approximations which might be relaxed at a later date although in general spraying is avoided in winds above 5m/s.

The governing differential equation (1) can be solved numerically to obtain the velocity of a droplet when it reaches the crop. Figure 1 shows the downward speed of various size droplets upon reaching the crop, assuming the initial conditions given above. The slope of the curve is shallower for droplets with a diameter below approximately 160μm. These are the droplets that reach terminal velocity before impacting on the crop at 50cm. For droplets larger than this diameter, the droplets do not have time to decelerate to terminal velocity before impacting with the crop. For example, a 700μm droplet takes 38ms to reach the crop. During this short time interval it decelerates from 15m/s to an impact speed of 11.6m/s, which is still much larger than its terminal velocity of 3.16m/s.

2.3. The simulation of a spray nozzle

There are many and varied nozzles used in spray applications, and spray nozzles used in boom spraying can produce a wide range of spray angles. A typical spray angle used in many applications is 80°. A simplified two-dimensional simulation of a nozzle with an 80° spray angle has been produced by releasing individual droplets, with initial speed 15m/s, at various angles $-130^\circ \leq \alpha \leq -50^\circ$ (where α is the angle above the horizontal). The components of the initial velocity of any given droplet are then given by $(15\cos\alpha, 15\sin\alpha)$. This simulation has been done for a variety of different droplet sizes and gives an idea of the trajectory of the droplets from the spray nozzle.

As the air is still, droplets travelling at terminal velocity are therefore falling vertically with the settling speed S, which is given in Table 1. We know from Figure 1 that 100μm droplets do reach terminal velocity before impacting, this can be clearly seen in Figure 2, the droplets are falling vertically upon impact on the plant which is at zero vertical

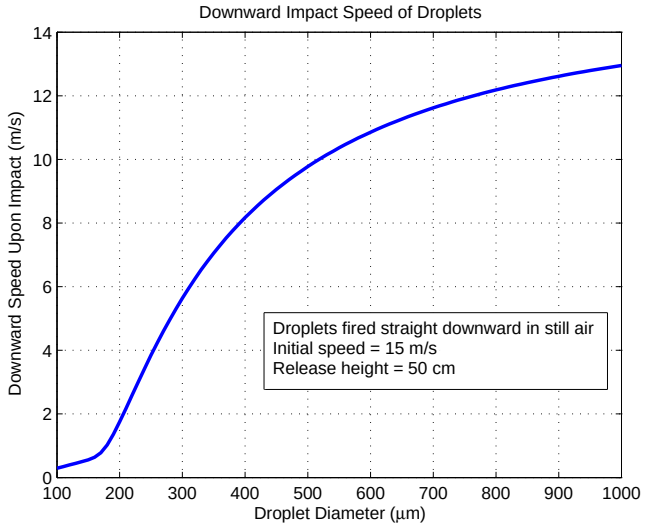

Figure 1. The impact speed of droplets with diameters ranging between 100μm and 1000μm. (The droplets have an initial velocity of 15m/s vertically downward and the crop is 50cm below the nozzle.)

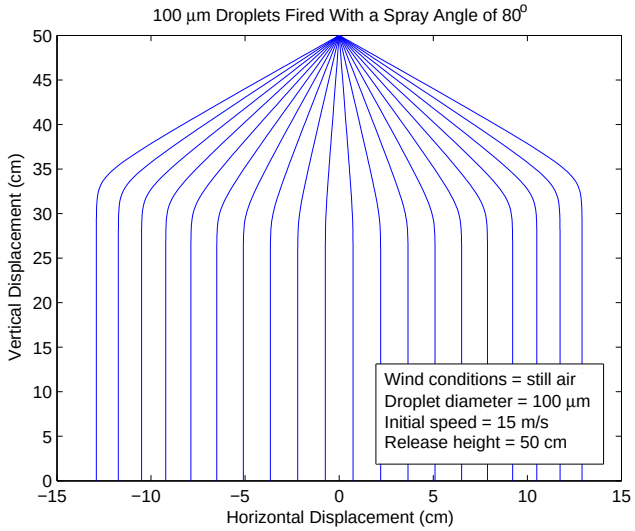

Figure 2. A two-dimensional simulation of the spray trajectory from a nozzle producing 100 μm droplets.

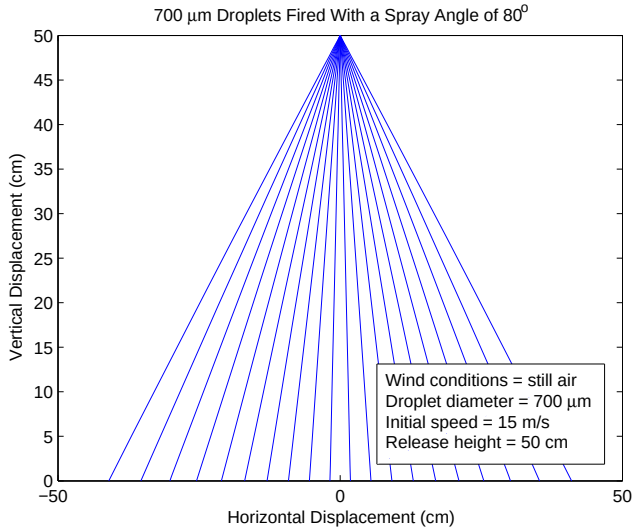

Figure 3. A two-dimensional simulation of the spray trajectory from a nozzle producing 700μm droplets.

displacement. However, this is not the case for droplets with diameter larger than approximately 160μm. The two-dimensional simulation of a nozzle producing 700μm droplets, again with an 80° spray angle, is shown in Figure 3.

We know from Figure 1 that 700μm droplets do not reach terminal velocity before impacting on the leaf surface at 50cm below the nozzle. In fact they lose comparatively little of their vertical velocity. From Figure 3, it can be seen that, at impact, these droplets also retain much of their initial horizontal velocity too. Therefore these 700μm droplets strike the plant canopy at an angle, not vertically as for the 100μm droplets.

In summary, droplets reaching the plant canopy will have a wide range of velocities dependent on their diameter. Small droplets will impact relatively slowly and vertically, while large droplets will impact much more rapidly, and at an angle. For a given nozzle with known velocity and droplet size distribution it is possible to determine the velocity (speed and angle) of each droplet when it impacts on the leaf surface at a given distance from the spray nozzle. This information is required for input into the retention models discussed in the next section.

3. Collision Models

3.1. Introduction

When a droplet impacts on a leaf surface it can do one of three things: adhere to the leaf; bounce off the leaf; or shatter into smaller droplets that may or may not adhere to nearby leaf surfaces. The factors that govern which behaviour results from an impact are the droplet size and velocity, the formulation of the droplet (whether surfactants have been added to alter the surface tension) and the leaf characteristics (such as wettability, angle and roughness). In this section models will be developed to describe whether or not a droplet impacts on a leaf and, if it does, what is the resulting behaviour. A similar collision model developed by Spillman [21] was used in the 2001 Mathematics in Industry Study Group to investigate the application of pesticide to grape bunches [2]. The model used here, and described below, is based on the Spillman [21] model with further refinements based on experimental validation.

3.2. Inertia Effects

Firstly, it must be determined whether or not droplets embedded in an air stream flowing directly towards a leaf will impact on the leaf surface or avoid it. This will depend on the size and velocity of the droplet. From studying droplet size distribution data provided by the industry representatives it was ascertained that here we are typically dealing with droplets with diameters (d) from 100μm to 1000μm. As fluid flows around a leaf small droplets are swept up with the flow and can possibly miss the leaf while larger droplets with more inertia will deviate from the flow and are more likely to impact on the leaf surface, see Figure 4 for a schematic diagram of this. Peters and Eiden [19] derived an empirical formula for the efficiency E of this impaction,

$$E = \left(\frac{\mathrm{St}}{\mathrm{St} + 0.8} \right)^2 , \tag{4}$$

based on the the Stokes number, St, of the flow

$$\mathrm{St} = \frac{\rho d^2}{18 \rho_a \nu_a} \frac{2U}{d_e} , \tag{5}$$

where U is the velocity of the droplet, d_e the diameter of the leaf as seen by the airflow, ρ_a the density of the air and ν_a the kinematic viscosity of air. Figure 5 shows the efficiency of impaction of the smallest droplets (100μm) for two leaf diameters (10mm and 50mm) as a function

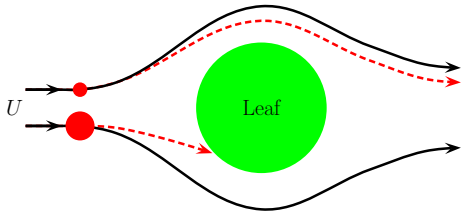

Figure 4. Large particles are possibly carried by their inertia into the leaf whereas lighter particles more closely follow the flow and may avoid the leaf surface.

of the droplet velocity. Even for the worst case scenario, of the smallest droplets under consideration and the largest leaf diameter, there is at least a 90% impaction efficiency for the droplet velocities that we are interested in. For the range of droplet sizes and velocities relevant to the problem under consideration, the vast majority of the spray impacts on the leaf surface, and so determination of these inertia effects is unnecessary in future calculations.

3.3. Adhesion or Bounce

When a droplet impacts a leaf surface its kinetic energy causes it to spread across the leaf surface. In doing so the kinetic energy is transferred to potential energy that is stored in the interface due to surface tension. As the droplet spreads it also loses energy due to friction. The droplet reaches a maximum spread and then begins to recoil back towards its original shape. See Figure 6 for a schematic representation of this mechanism. If the energy losses are small enough the droplet will reform and detach from the leaf surface. If the losses are large enough then the droplet recoil is insufficient to reform the droplet and it will remain attached to the leaf surface. The factors affecting this process are the droplet size and velocity (influencing the kinetic energy), the surface tension of the droplet formulation, the advancing and receding angles of the droplet over the surface, the wettability of the surface, the surface roughness and the friction coefficient.

Following Pasandideh-Fard *et al.* [17] (and others such as Mourougou-Candoni *et al.* [14], Yoon *et al.* [24]) an equation for the maximum spread of a droplet can be determined. For an initially spherical droplet of diameter d, density ρ and velocity v the kinetic energy is

$$KE = \frac{\pi}{12}\rho v^2 d^3 \tag{6}$$

and the surface energy is

$$SE_i = \pi d^2 \gamma \tag{7}$$

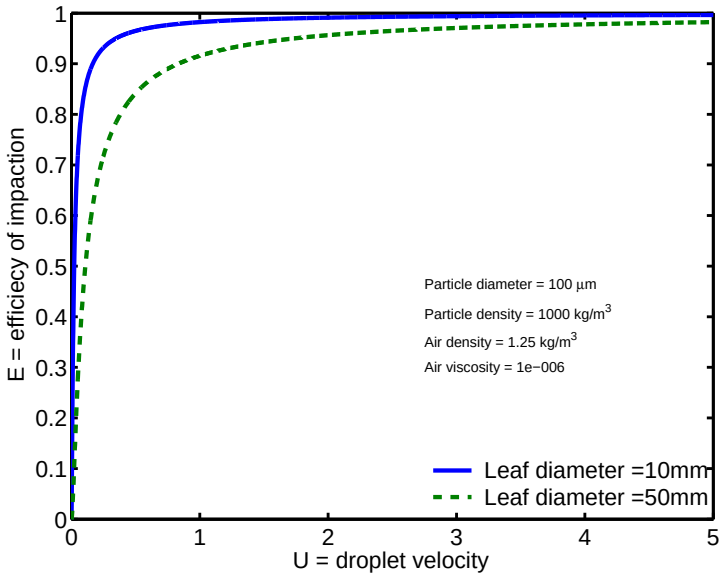

Figure 5. Impaction efficiency versus droplet velocity (in m/s) for two leaf diameters ($d_e = 10$ and 50 mm) with the smallest droplet diameter of interest (100μm).

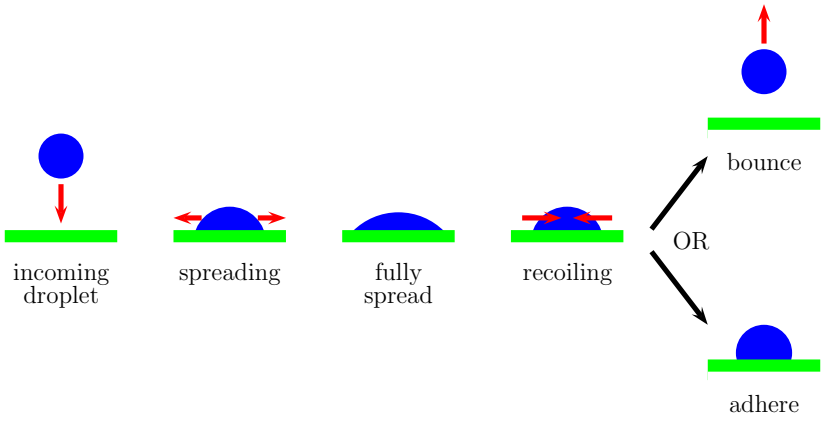

Figure 6. Schematic diagram of the spread and recoil of a droplet showing the two possible scenarios of adhesion and bounce.

where γ is the equilibrium surface tension of the formulation. The subscript i refers to the initial surface energy and later the subscript f refers to the surface energy at full extended position. When the droplet reaches its fully spread extent it is assumed to be a thin pancake-shaped layer of diameter d_{max}. The kinetic energy is zero. By subtracting the effect due to the wetting of the leaf surface by the bottom of the droplet from that due to surface tension in the droplet's free top surface, the effective surface energy is

$$SE_f = \frac{\pi}{4} d_{max}^2 \gamma (1 - \cos\theta_A) \tag{8}$$

where θ_A is the advancing contact angle of the droplet on the leaf surface (this depends upon the leaf type and formulation). The work done in deforming the droplet against viscosity is shown in Pasandideh-Fard *et al.* [17] to be

$$WD = \frac{\pi \rho v^2 d d_{max}^2}{3\sqrt{Re}} \tag{9}$$

where $Re = vd/\nu$ is the Reynolds number of the flow and ν is the kinematic viscosity of the formulation. Figure 7 shows energies associated with the combinations of two different sizes of droplet and two different liquid formulations. The two droplet diameters are 1000μm ((a) and (b)) and 100μm ((c) and (d)). The liquid formulations considered are water, which has a contact angle of 110° and a surface tension of 0.072Nm, ((a) and (c)), and water with a surfactant added, for which the contact angle reduces to 30° and the surface tension reduces to 0.032Nm ((b) and (d)). [9] For both droplet sizes adding the surfactant increases the work done in the spreading phase as the droplet spreads further across the leaf surface. Also the surface energy at full spread (SE_f) is lower and hence there is less energy stored in the droplet so recoil and bounce is less likely to occur.

Using energy conservation from the incoming droplet and up to the point of maximum spread

$$KE + SE_i = SE_f + WD \tag{10}$$

and rearranging gives the maximum spread factor as

$$\beta = \frac{d_{max}}{d} = \sqrt{\frac{We + 12}{3(1 - \cos\theta_A) + 4\,We/\sqrt{Re}}} \tag{11}$$

where $We = \rho d v^2/\gamma$ is the Weber number, a measure of the balance between the inertial and capillary forces. This formula for the maximum spread gives good agreement with experimental and detailed numerical

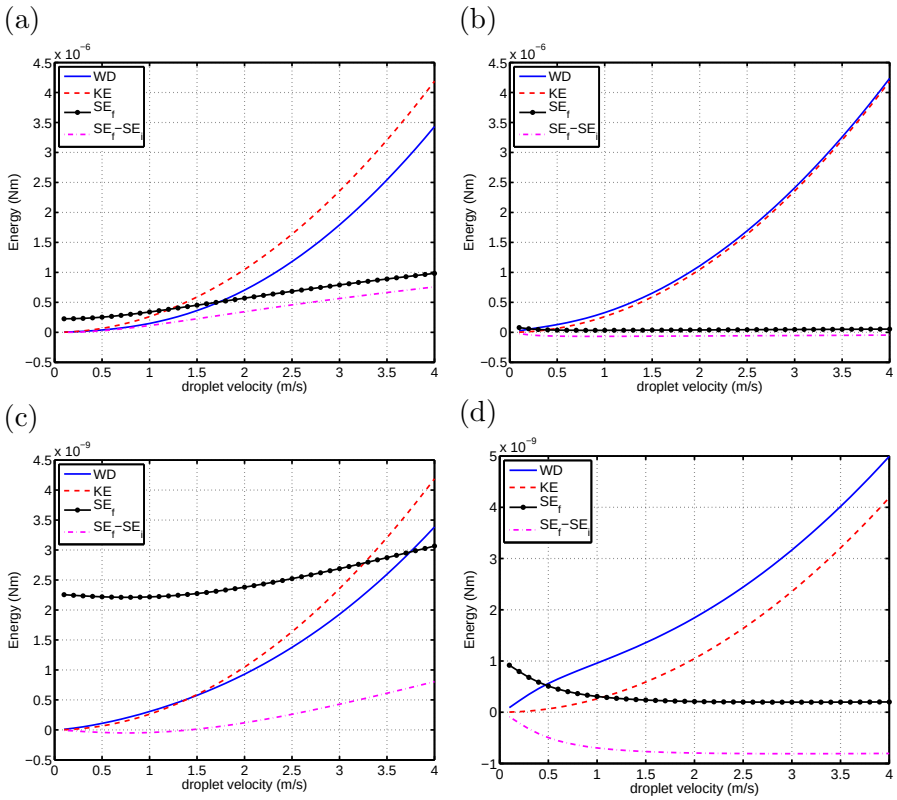

Figure 7. Energies of a 1000μm droplet ((a) and (b)) and a 100μm droplet ((c) and (d)) before impact (KE and SE_i) and at maximum spread (WD and SE_f). (a) and (c) are for water with a contact angle of 110° and surface tension γ=0.072Nm. (b) and (d) are for water with a surfactant added so lowering the contact angle to 30° and surface tension to γ=0.032Nm.

investigations as outlined in Pasandideh-Fard *et al.* [17]. They found that the advancing contact angle was a good measure of the effect of adding a surfactant to the droplet formulation. (A surfactant generally decreases the contact angle by increasing the wettability of the formulation and lowering its surface tension.) Of particular interest is that the equilibrium surface tension was found to correlate better with the maximum spread as compared to the dynamic surface tension. An explanation of this is that the time scale for the dynamic surface tension to change is a lot greater than that for the droplet to spread: it is of the order of 200ms (Forster *et al.* [8]) compared to 20ms (Pasandideh-Fard *et al.* [17] and Mourougou-Candoni *et al.* [14]). In contrast to this, the experimental work of Forster *et al.* [8] has shown that dynamic surface tension is well correlated to spray retention. This is not contradictory as Crooks *et al.* [6] show that there is a critical surfactant concentration below which dynamic surface tension is not a factor in the droplet spread and above which it is a dominant factor. Dynamic surface tension is more likely to have an impact in the recoil phase of a droplet's motion and hence can indeed be related to the ultimate retention of the droplet on the leaf surface. Experiments conducted by Webb and Holloway [23] show that formulations with a lower dynamic surface tension are retained after fewer bounces and also can have a higher impact velocity before bounce of the droplet occurs. These factors have implications for the interpretation of both experimental and analytical results.

Determining whether a droplet adheres or bounces from the leaf surface is more difficult that just calculating the maximum spread of the droplet and the energy lost in that spread. The droplet will also lose energy on recoil but this is more difficult to determine and, according to Yoon *et al.* [24], as yet no relationships have been found. There have been some attempts to quantify this, with Aziz and Chandra [1] suggesting from experimental evidence of small ($< 80\mu m$) droplets of molten metal that the droplet will bounce if $SE_f > WD$. However, there is no physical justification of this and it is contrary to other evidence. Further, this assumes that the energy lost in the recoil phase is equivalent to that lost in the expanding phase which is clearly untrue, as the recoil velocity is substantially less than the expanding velocity as noted by Bergeron *et al.* [3]. Droplets may in fact bounce multiple times at the leaf surface [23]. This can affect retention as a multiple bouncing droplet may still be retained on the leaf surface. In fact, if droplets are going to bounce off and escape from the leaf surface completely, this will generally happen at the first bounce. To determine an approximate criteria for droplet bounce consider the total energy available in the droplet for the recoil phase. For a given droplet diameter at maximum spread extent,

the droplet has a total energy equal to the surface energy SE_f. For the droplet to reform it must have an amount SE_i of that quantity retained as a surface energy when the droplet leaves the leaf surface, so the total available energy to be lost on the recoil phase is $SE_f - SE_i$. This is shown in Figure 7 as the dot-dash line. If the recoiling drop leaves the leaf with a kinetic energy KE_b then

$$KE_b + WD_r = SE_f - SE_i \ (= KE - WD). \tag{12}$$

Assume that the energy lost in the recoil phase (WD_r) follows the same physical mechanism (but at a lower velocity [3]) as that lost in the spreading phase. (This is not exactly true as spread and recoil are different mechanisms but it is likely to be approximately correct.) From Figure 7 it is then possible to determine if bounce can occur. For a given incoming droplet velocity (v) determine the available energy for recoil ($SE_f - SE_i$) and equate this to the energy for work done (WD_r) (draw a horizontal line from the $SE_f - SE_i$ curve to the WD curve). Now determine what surrogate velocity this gives the droplet. If at that surrogate velocity the kinetic energy (KE_b) is less than the work done then there is not sufficient energy for the droplet to reform and leave the leaf surface. That is, all the available energy has been used in the droplet recoil phase and so it adheres to the surface. The point where the kinetic energy equals the work done therefore gives the critical value of available energy for the recoil phase which in turn gives the critical incoming droplet velocity where bounce is possible.

To clarify this consider the example of a 100μm droplet with a contact angle of 110° and a surface tension of 0.072Nm travelling at 4m/s. From Figure 7(c) this has approximately $SE_f - SE_i = 0.8 \times 10^{-9}$Nm of energy available to be lost on the recoil phase. The critical assumption is that the energy loss on recoil is by the same mechanism as expansion just at a lower velocity so find the velocity of a surrogate droplet that loses that much energy during the expansion phase. For that amount of energy the surrogate velocity is given by the WD line on Figure 7(c) as approximately 1.8m/s. So the amount of energy loss is equivalent to a surrogate droplet coming in at 1.8m/s and expanding. For such a surrogate droplet the kinetic energy is larger than the energy lost (the KE line is above the WD line). Hence not all of the energy available to the original droplet at its fully expanded position is lost on recoil and so that droplet will have some energy left at the point where it reforms as a sphere which is converted to kinetic energy and the droplet bounces off of the leaf surface. To find the critical value consider a droplet with incoming velocity of approximately 3.3m/s. At this velocity the available energy $SE_f - SE_i$ is approximately 0.55×10^{-9}Nm. This corresponds

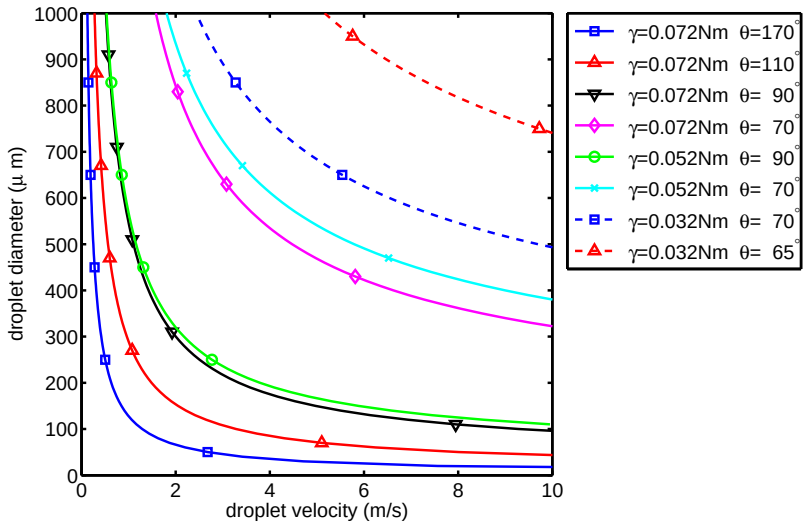

Figure 8. The boundary between droplets adhering to the surface and bouncing off for various surface tension and contact angles. Below a line the droplets adhere and above a line the droplets will bounce.

to a surrogate velocity of approximately 1.45m/s. At this surrogate velocity WD is equal to KE so the surrogate droplet would expend all its available energy in the expansion phase. By the assumption this means that the original droplet will just expend all its available energy on the recoil phase and not bounce off the leaf surface.

Shown in Figure 8 is a plot of this critical adhere/bounce line as droplet diameter versus incoming droplet velocity for various contact angles and surface tensions. Points below the lines correspond to droplets adhering and points above the lines to droplets bouncing (and potentially not adhering). As the surface tension and contact angle are decreased, droplets are more likely to adhere to the leaf surface. For example consider a 400μm droplet travelling at 1m/s. If the droplet has a surface tension of 0.072Nm and a contact angle on the leaf surface of 170° then it will bounce. In contrast on a different leaf type this droplet may have a contact angle of 90° in which case it will adhere to the leaf surface.

Further work is needed in this area. The formulae need to be compared with experimental results to see if just surface tension and contact angle are adequate to describe all the known behaviour. It is suspected that leaf surface roughness will have an active part to play in the droplet spread and this may need to be incorporated into the theory. Dynamic

surface tension is known to correlate well with retention and the effect of that should also be investigated. Throughout we have assumed that the leaf is horizontal and the droplet is moving vertically. It is well known that the retention rate changes with leaf angle [9] and this needs to be investigated using these formulae. It is expected that the component of the velocity normal to the leaf surface will be the critical incoming velocity but this will need to be verified experimentally. Throughout this work it has been assumed that the viscosity of the formulation (as it appears in the Reynolds number) is not altered. Mao *et al.* [13] have shown that "the tendency of droplets to recoil and rebound is less for higher viscosity liquids than for lower viscosity liquids", hence any changes in viscosity brought about by the addition of a surfactant should also be included in a model. Recent work by Bergeron *et al.* [3] has shown that the inclusion of a small amount of polymer additive can drastically alter the recoil characteristics. Although out of the scope of the present project this is an area that requires further analytical and experimental work.

3.4. Shatter

When a droplet strikes a leaf in a more energetic state than for the bounce mode described above it is also possible for it to break up into many smaller droplets. We will call this behaviour shattering of the droplet. It is also known as splashing or droplet breakup. In the context of spray retention, this shattering is not necessarily a bad outcome as the droplet breaks into smaller, slower-moving droplets that are more easily captured on nearby leaf surfaces and can actually enhance the retention of the spray.

In a similar manner to that described above for the bouncing of droplets, Mundo *et al.* [15] considered energy balances and derived a criteria for the splashing of droplets as

$$We^2\, Re > K^4 \tag{13}$$

where K is a constant. Mundo *et al.* [15] found this constant to be $K = 57.7$ over a wide range of substrate (leaf) roughness ranging over $0.001 < \mathcal{R} < \infty$ where $\mathcal{R}$ is a nondimensional roughness and defined as the ratio of the surface roughness to the droplet diameter[16]. Yoon *et al.* [24] discuss this constant and note that "K increases with decreasing surface roughness since an impacting liquid droplet can spread further on a smooth surface before it shatters". They show that for the experiments of Mao *et al.* [13] the value of K can be up to $K \approx 152$ for water on a paraffin wax surface. Shown in Figure 9 are plots of equation (13) for 3 different surface tensions ($\gamma = 0.072$, 0.052 and 0.032Nm) and 3

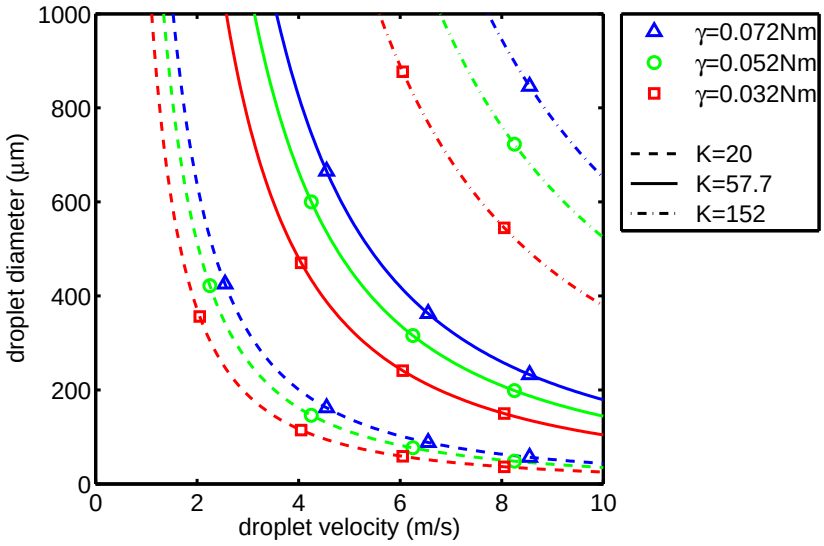

Figure 9. Boundary between droplets shattering on impact with the surface and bouncing/adhering to the surface for various surface tensions and values of the constant K in equation (13). Above a line the droplets shatter on impact and below a line the droplets will bounce/adhere.

values of the constant K (20, 57.7 and 152) to cover a wide range of different surface types. Above a line the droplet shatters and below a line it either bounces or adheres as given by the previous section. As K decreases the critical shatter velocity of a given droplet size decreases, so for rough leaf surfaces the velocity above which shattering occurs is lower than for smoother leaf surfaces. As the surface tension decreases, the critical shatter velocity of a given droplet size decreases as there is less surface force holding the droplet intact. Adding a surfactant increases the likelihood of shatter which is beneficial to retention of the spray on the leaf surface.

Further analytic work is needed in this area to incorporate the surface roughness and contact angle into the formulae so that a predictive value of K can be determined. At present, the value of K that is relevant to a particular leaf type and formulation must be determined experimentally. The result given by equation (13) needs further experimental work to determine its usefulness in real world applications although it does show great promise as a predictive tool for droplet shattering.

4. Run–off

4.1. Introduction

When a solid surface is sprayed, the drops adhering to the surface increase in size as more spray droplets impact upon them and they coalesce with neighbouring drops. The amount of spray retained on the surface grows until the surface drops grow to a critical size, above which they begin to slide down the surface and drip off. This is called run–off. Further spraying usually increases run–off and the maximum retention is at the point of run–off. Any spraying done past the point of runoff is potentially wasteful and so an estimate of this point is keenly sought after by the industry.

According to Furmidge [10] the surface properties of the spray liquid/solid combination are among the most important factors determining spray retention on solid surfaces. He developed a theory of how the physical properties of the spray liquid and the solid surface govern retention and then determined theoretical retention figures for different spray formulations. This theory will be summarised here.

4.2. Determining the angle for run-off

Furmidge [10] studied the sliding of drops of water and solutions of surfactants on wax and cellulose acetate surfaces. This is a static situation where the movement of a drop is expressed in terms of the droplet size, the angle of tilt of the surface, the surface tension of the spray liquid, and the advancing and receding contact angles of the droplet.

For a given liquid on a given surface, several authors have produced the following expression:

$$\frac{mg\sin\alpha}{\omega} = H_\gamma, \tag{14}$$

where m is the mass of the drop on the surface, α is the angle of tilt of the surface necessary to start sliding of the drop, γ is the surface tension of the drop (determined by the spray formulation), and ω is the width of the drop on the leaf. H_γ is a constant that varies only with the droplet surface tension and not the leaf angle and so can be determined from a single measurement.

As the proportion of surfactant in the spray solution increases, the angle at which run–off will occur decreases across the range of droplet widths, as seen in Figure 10 which is a comparison of the sliding angle at two different surfactant levels. Note that as surfactant is added the size of a droplet that can be supported on a vertical leaf (90° sliding angle) is decreased.

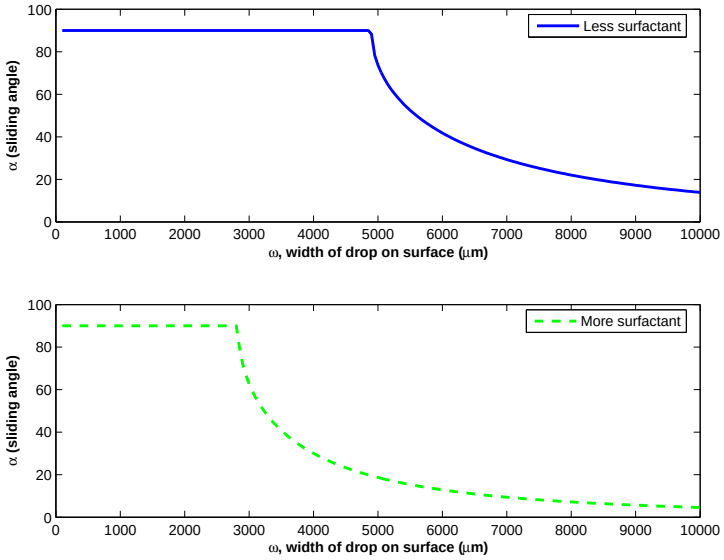

Figure 10. Relationship between droplet size and the angle of tilt required for run-off for different quantities of surfactant in the spray solution.

The droplet on the leaf surface does not stay spherical but rather forms a spherical cap of width ω proportional to the width of the sprayed droplet, d. Using volume formulae for the spherical cap and sphere we can determine d in terms of ω as

$$\frac{\pi}{6}d^3 = \frac{\pi(1-\cos\theta)^2(2+\cos\theta)}{24\sin^3\theta}\omega^3, \tag{15}$$

where θ is the contact angle of the spherical cap with the leaf surface. Rearranging gives

$$d = \frac{1}{\sin\theta}\sqrt[3]{\frac{(1-\cos\theta)^2(2+\cos\theta)}{4}}\,\omega. \tag{16}$$

For example, if the contact angle of the drop with the surface is 60°, then we have $d \approx \frac{3}{5}\,\omega$.

4.3. The sliding of drops

The force that causes the drop to move is $mg\sin\alpha$ and so the work done by the drop in descending a distance l is $W = lmg\sin\alpha$. The work done in overcoming surface tension while moving a distance l is given by $W = \gamma\omega l(\cos\theta_R - \cos\theta_A)$, where θ_A is the advancing contact angle of the drop and θ_R the receding contact angle as shown in Figure 11. By

equating these two different expressions for the work done we obtain

$$W = lmg \sin\alpha = \gamma\omega l(\cos\theta_R - \cos\theta_A), \tag{17}$$

and using equation (14) gives

$$\gamma(\cos\theta_R - \cos\theta_A) = H_\gamma. \tag{18}$$

This formula gives a constant relating the spray formulation (given by γ) and the leaf surface (given by θ_A and θ_R) and can be used in developing a theoretical retention formula. As has been indicated above, the benefit of the formula is that H_γ can be found from one experiment at one leaf angle and then the formula can be used at other leaf angles. Many of the physical characteristics of the leaf (wettability, roughness etc.) are incorporated in this constant H_γ and hence do not need to be measured. This constant varies from leaf type to leaf type so each leaf type needs a different experiment but only at one angle.

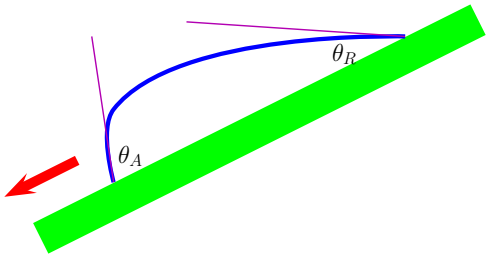

Figure 11. Schematic diagram of a drop sliding down a surface showing the advancing angle (θ_A) and the receding angle (θ_R).

4.4. Spray retention

Using (18) and following Furmidge [10] a retention formula can be derived for a continuous steady spray onto a leaf up to the point of loss of retention as

$$R = k\sqrt{\left(\frac{\pi\gamma(\cos\theta_R - \cos\theta_A)}{24\rho g \sin\alpha}\right)}\sqrt{\left(\frac{(1-\cos\theta_A)^2(2+\cos\theta_A)}{\sin^3\theta_A}\right)}. \tag{19}$$

where k depends upon the spray droplet spectrum and is approximately constant for most spray/surface combinations [10]. The equation shows that retention is governed by the surface tension of the spray fluid, the difference of the advancing and receding contact angles and the value of the advancing contact angle of the sprayed liquid on the solid surface.

Figure 12 shows a comparison of the retention of water on to two different surfaces (differentiated by having different θ_A and θ_R) as the angle of the leaf (α) is varied.

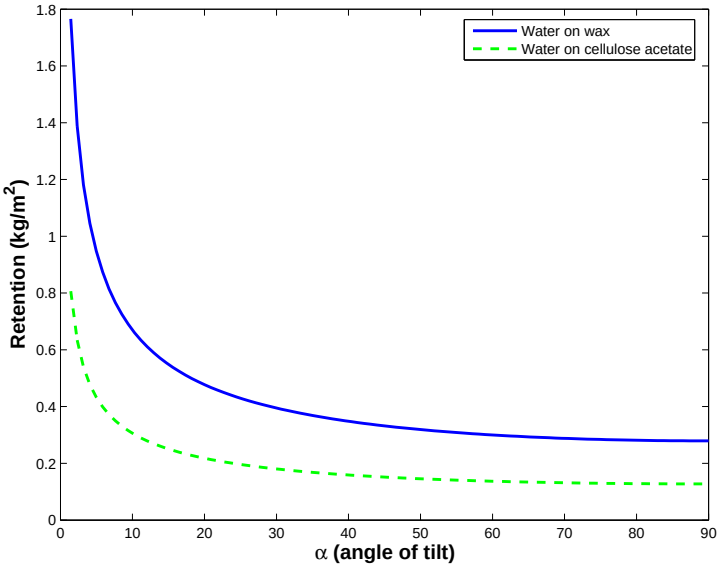

Figure 12. Changes in theoretical retention for water on two different surfaces with varying angle of tilt.

By defining θ_M as the arithmetic mean of θ_A and θ_R, a retention factor is derived which can predict with reasonable accuracy the relative order of retention found in practice as

$$F = \theta_M \sqrt{\gamma(\cos\theta_R - \cos\theta_A)/\rho}. \tag{20}$$

This formula is not a measure of the absolute retention onto a leaf surface but is rather used to rank different formulations. A larger F means that the particular combination of formulation (given by γ and ρ) and leaf type (given by θ_A, θ_R and θ_M) will retain more spray than another combination with a smaller F. The power of this approach is that very small numbers of experiments need to be undertaken to be able to rank the retention capabilities of different formulations on different leaves, with few physical parameters required. The details of this and how it is implemented in their experimental retention work is left to the industry partner.

5. Plant Canopy Models

5.1. Introduction

Ray-tracing models can be used to estimate droplet retention. A basic two-dimensional model using L-systems to represent branches and with a separate model for leaves is described here.

Some more sophisticated versions of this approach have already been developed [20]. These systems are also being used to determine rainfall inception and subsequent water infiltration and run-off in soils [4]. Within Australia, a report of work done by the Centre for Plant Architecture at the University of Queensland, [5], and [7] shows how L-systems are being used to model various plant structures.

5.2. Branch model using L-systems

L-systems originated with A. Lindenmayer [12] for modelling multicellular organisms that form branching filaments. L-systems are recursive representations which involve a series of symbols for graphical instructions for drawing the branch structure. As an example, we consider the following string:

$$F[+G][-G]F[+G][-G]FG \tag{21}$$

Here F and G correspond to line segments, of different lengths, $+$ means turn by an angle θ and $-$ means turn by an angle $-\theta$. The [ ] notation indicates a specific branch; when that branch is drawn you return to the original coordinate. An example of the structure drawn by these commands is shown in Figure 13. In this example length$(F) = 1$, length$(G) = 2$, and $\theta = 27.5°$.

An iterative rule is defined, which is then applied recursively. For example, consider the rule

$$F \to FF \tag{22}$$

$$G \to F[+G][-G]F[+G][-G]FG \tag{23}$$

Applying this rule once recursively to equation (21) gives the more complicated drawing instruction

$$FF[+F[+G][-G]F[+G][-G]FG][-F[+G][-G]F[+G][-G]FG]$$
$$FF[+F[+G][-G]F[+G][-G]FG][-F[+G][-G]F[+G][-G]FG]F$$
$$FF[+G][-G]F[+G][-G]FG$$

with the graphical representation shown in Figure 13. A variety of branching structures can be obtained by changing the string, the rules and the number of recursion steps.

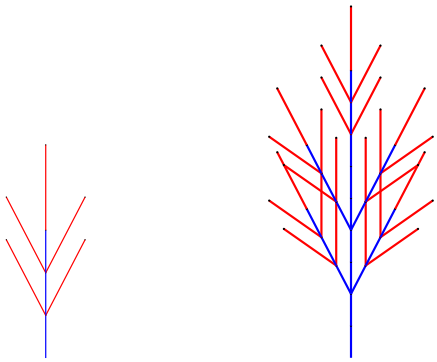

Figure 13. On the left, the graphic defined by the string $F[+G][-G]F[+G][-G]FG$ which corresponds to one application of the rule. Here F (blue) and G (red) correspond to line segments of length 1 and 2, respectively, and in both cases with the angle $\theta = 27.5°$. On the right is the graphic obtained by applying the rules (22,23) once recursively.

5.3. Leaf model

To be able to model retention leaves need to be placed on the branches. In modelling real plant structures this is done in such a way as to mimic the plant leaf characteristics such as angle, size, clumping, etc. For the sake of simplicity, here, in this two-dimensional model, leaves are modelled as planes with a random orientation to the horizontal. These orientations are chosen from a uniform distribution between angles of $\pm\alpha$. In Figure 14, a graphical representation of the leaves and branches is shown with $\alpha = 45°$.

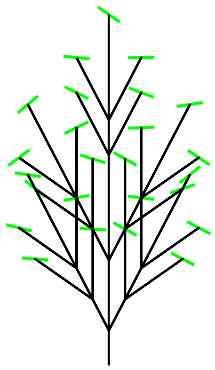

Figure 14. A model of a plant canopy including leaves modelled as planes with an orientation chosen randomly from a uniform distribution between the angles of $\pm 45°$ to the horizontal.

5.4. Ray tracing analysis

To investigate droplet retention we employ a ray-tracing approach. As a first model, we assume the droplet falls vertically and if the droplet path intersects with a leaf then it is retained by the leaf. This is easily implemented in a Matlab computer program.

In Figure 15, the percentage retention of droplets is shown for a sequence of realisations of the model with increasing leaf size. Generally, as the leaf size increases the overall droplet retention percentage increases towards 100%. Note that, because of the random distribution of leaf orientations in each realisation, it is possible for a small increase of leaf size in the model to correspond to a small decrease of retention percentage in the realisation of the model. Also shown is the percentage retention of the plant canopy assuming that each individual leaf only retains 75% of the droplets which impact upon its surface.

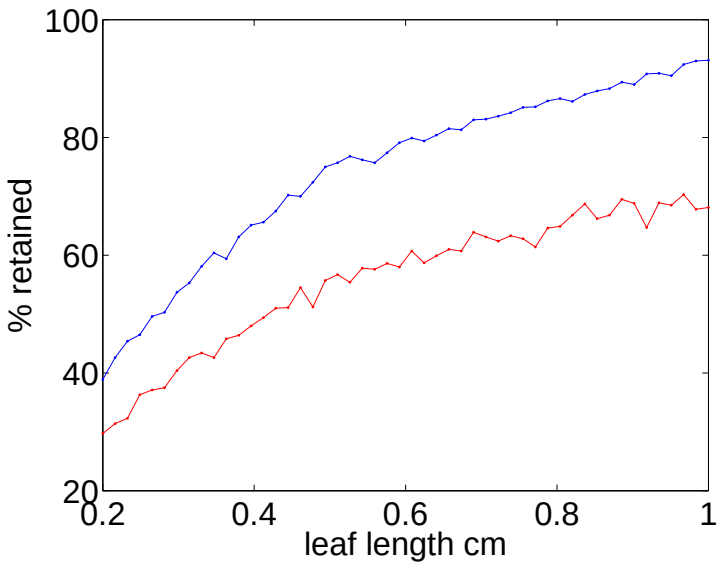

Figure 15. Percentage droplet retention for the whole branch and leaf model of Figure 14 as the leaf length is increased. The upper line assumes 100% retention while the lower line assumes 75% retention for each impact on an individual leaf.

The model described here is clearly simplistic, but it does illustrate a general approach which may be developed further. In particular the model may be extended to three dimensions [22] and more realistic leaf models can be incorporated [20]. The conclusions of the earlier work on droplet adhesion, bounce, shatter and retention on individual leaves can

be incorporated. For example, the droplet retention probability could depend on the amount of droplets already retained.

6. Stochastic Models

6.1. Introduction

The ultimate aim of this project is to have a comprehensive model that enables the prediction of spray retention on plant leaves when given inputs such as the formulation used, the spray nozzle (droplet and velocity distribution) and type of crop. By compartmentalising each physical process, as outlined in the sections above, this is possible. We have developed models for the spray trajectory, the impaction on the leaf, the retention and the canopy structure. Each of these sections can be validated by experimental work and refined as the individual models are improved. In this section the elements discussed in the previous sections are combined in a stochastic model to give an indication as to how this type of comprehensive model may be progressed. The work presented below is not the definitive model as that is beyond the scope of the current project, rather it is an indication of the direction in which these types of models can be developed.

6.2. A first simple model

The following model considers each droplet individually through a number of decisions as to the droplet's fate. Firstly, given a droplet's size and velocity as it leaves the spray nozzle, its velocity at the canopy can be derived from Section 2. The decision is then whether the droplet will hit a leaf or miss. This occurs with probability, P, depending on the structure of the canopy. This probability can be derived from Section 5 type models. For the sake of this example, if the droplet does hit the leaf, the angle, θ, it strikes its surface is randomly sampled from a normal distribution with mean 45° and standard deviation of 10° (samples are rejected if $\theta > 90$ or $\theta < 0$), that is the spray is incoming at an angle of approximately 45° to the leaf. In general the angle of incidence can be determined from the droplet's trajectory and from the canopy models that give the leaf angles for each different crop type.

The next decision is whether the droplet shatters, adheres or bounces on impact with the leaf. This is determined by the collision models developed in Section 3. The effect of run-off considered in Section 4.1 could also be incorporated at this stage, although it is not included in this first simple model. Here shattered droplets are assumed to be retained, as the resulting smaller droplets will stick to any leaf they come

into contact with. If the droplet does not shatter it either sticks to the leaf and is retained or it bounces. If a droplet bounces then it may be captured by either landing on the same leaf again, with probability $1 - P(\text{bounce})$, or by bouncing off the leaf and hitting another with the same probability, P, as in the initial decision. Actually, the true probability, P', will be less than P as the droplet has already passed partially through the canopy. Here any droplet that bounces and hits another leaf is assumed to be retained as its velocity will have been substantially reduced by the initial collision. This is validated by Figure 7 where the energy of droplets that bounce off is seen to be substantially reduced so that they do not have enough energy to bounce off a subsequent leaf they may impact upon. This decision process is shown schematically in Figure 16.

These types of models can be run numerous times with the stochastic nature being realised in the distributions of the leaves in the canopy models and the incoming spray trajectory. Typical capture results for this type of model are shown in Figure 17. In this illustration the model has been run 100000 times with 1000 different droplets each time and the capture count of each droplet size determined. When the method is fully implemented these types of figures will be useful in showing the optimal droplet size distribution to use in a given scenario. The spray operator would then be able to choose their sprayer to operate in this region.

Ultimately it is possible to develop software that incorporates each of these compartment models into a comprehensive spray retention model. By doing this in a modular fashion each component can be individually validated experimentally and improved upon as better component models are developed. It should be reiterated here that this model is not a definitive retention model at this stage but rather an example of how such models can be constructed and assembled in the future.

7. Conclusion

In the course of this project the MISG group reduced the process of spray retention on plants into a number of sub problems. Each of these was successfully tackled. Methods for determining the trajectory of the spray from the nozzle to the plant have been described, and these can be used as input into future plant canopy interception models. For the range of droplet sizes and velocities under consideration, it was shown that the inertia effects are not important, and that the majority of droplets will impact upon a leaf if it is upon their trajectory. Detailed models for the bounce, shatter or retention of droplets as they impact on a leaf surface

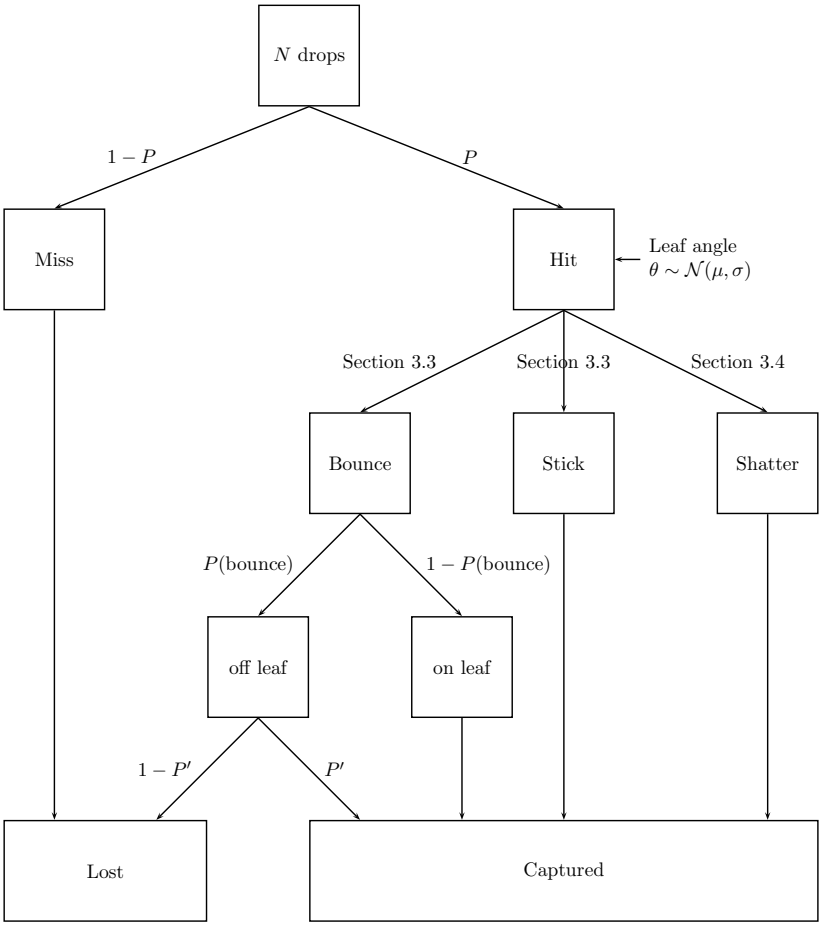

Figure 16. A schematic of the stochastic model. N droplets go through a number of decisions to decide whether they are captured or lost. The probability of an initial hit, P, can be derived from Section 5 type models and the probability of bouncing off the leaf is $P(\text{bounce}) = \min(1, 4|v|^2 \sin\theta/Lg)$, where L is leaf length, g is gravity and v terminal velocity.

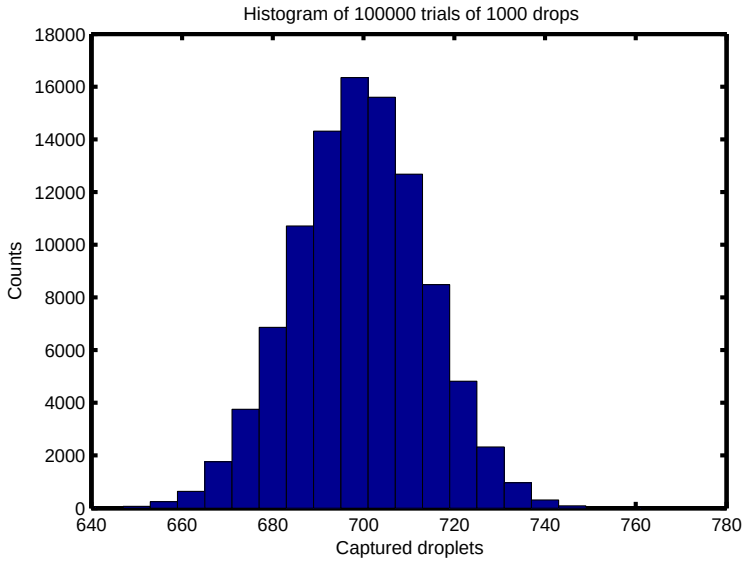

Figure 17. A sample capture result from running a typical model 100000 times with 1000 different drops.

were developed. Parameters of interest include the surface tension of the droplets, the surface roughness, the droplet size and velocity and the droplet contact angles. The industry partner is undertaking further research in this area. It has recently purchased equipment to measure droplet contact angles and is conducting experiments to validate some of the theoretical calculations. The MISG group investigated run off models and a means of ranking different formulations was determined. A preliminary investigation into plant canopy models and simulations of the interception of plants using the other models listed above was undertaken.

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References

[1] Aziz S.D.& Chandra S., "Impact, recoil and splashing of molten metal droplets", *International Journal of Heat and Mass Transfer*, **43** (2000), pp. 2841–2857.

[2] Barry S.I. & Weber R.O., "The application of pesticides to grape bunches", *Proceedings of the 2001 Mathematics in Industry Study Group*. Ed. J. Hewitt, (2002).

[3] Bergeron V., Bonn D., Martin J.V. & Vovelle L., "Controlling droplet deposition with polymer additives", *Nature*, **405** (2000), pp. 772–775.

[4] Busière F., Solmon F. and Fouéré A., "Implementation and evaluation of drop, a model for the simulation of rainfall distribution below plants described in 3d", *Agronomie*, **22** (2002), pp. 93–103.

[5] CPAI, Center for plant architecture informatics biennial report. Technical report, University of Qld, (2002).

[6] Crooks R., Cooper-Whitez J. & Boger D.V., "The role of dynamic surface tension and elasticity on the dynamics of drop impact", *Chemical Engineering Science*, **56** (2001), pp. 5575–5592.

[7] Dorr G. J., Hannan J., Woods N., Adkins S., Kleinmeulman P., Ricci P. and Noller B., "Combining spray drift and plant architecture modeling to minimise environmental and public health risk of pesticide application", Technical report, Centre for Plant Architecture and Systems, University of Qld, (2006).

[8] Forster W.A., Kimberley M.O., Steele K.D., Haslett M.R. & Zabkiewicz J.A.,"Spray retention models for arable crops", *Journal of ASTM International*, **3(6)** (2006), in press.

[9] Forster W.A., Kimberley M.O. & Zabkiewicz J.A., "A universal spray droplet adhesion model", *Transactions of the American Society of Agricultural Engineers*, **348(4)** (2005), pp. 1321–1330.

[10] Furmidge C.G.L., "Studies at Phase Interfaces, I. The sliding of liquid drops on solid surfaces and a theory for spray retention", *Journal of Colloid Science*, **17** (1961), pp. 309–321.

[11] Furmidge C.G.L., "Physico–Chemical Studies on Agricultural Sprays, IV. The retention of spray liquids on leaf surfaces", *J. Sci. Food Agric.*, **13** (1962), pp. 127–140.

[12] Lindenmayer A., Mathematical models for cellular interaction in development, parts i and ii.", *Theor. Biol.*, **18** (1968), pp. 280–315.

[13] Mao T., Kuhn D.C.S. & Tran H., "Spread and rebound of liquid droplets upon impact on flat surfaces", *American Institute of Chemical Engineers Journal*, **43(9)** (1997), pp. 2169–2179.

[14] Mourougou-Candoni N., Prunet-Foch B., Legay F., Vignes-Adler M. & Wong K., "Retraction phenomena of surfactant solution drops upon impact on a solid substrate of low surface energy", *Langmuir*, **15** (1999), pp. 6563–6574.

[15] Mundo C.H.R., Sommerfield M. & Tropea C., "Droplet-wall collisions: Experimental studies of the deformation and breakup process", *International Journal of Multiphase Flow*, **21(2)** (1995), pp. 151–173.

[16] Mundo C.H.R., Sommerfield M. & Tropea C., "On the modeling of liquid sprays impinging on surfaces", *Atomization and Sprays*, **8** (1998), pp. 625–652.

[17] Pasandideh-Fard M., Qiao Y.M., Chandra S. & Mostaghimi J., "Capillary effects during droplet impact on a solid surface", *Physics of Fluids*, **8** (1996), pp. 650–659.

[18] Perry R.H., Green D.W. & Maloney J.O., *Perry's Chemical Engineers' Handbook*, 6th Ed., (McGraw-Hill, 1984).

[19] Peters K. & Eiden R., "Modelling the dry deposition velocity of aerosol particles to a spruce forest", *Atmospheric Environment*, **26A** (1992), pp. 2555–2564.

[20] Prusinkiewicz P., *The Algorithmic Beauty of Plants*. Springer-Verlag, (1990).

[21] Spillman J., "Spray impaction, retention and adhesion: an introduction to the basic characteristics", *Pesticide Science*, **15** (1984), pp. 97–106.

[22] de Visser P. H. B., Marcelis L. F. M., van der Heijden G. W. A. M., Vos J., Struik P. C. and Evers J. B., "3d modelling of plants: a review", Technical report, Wageningen, Plant Research International B.V., (2002).

[23] Webb D.A. & Holloway P.J., "Low speed impact behaviour of aqueous monosize spray droplets containing agricultural additives on plant surfaces", *Proceedings of the 15th Annual Conference on Liquid Atomization and Spray Systems*,(1999).

[24] Yoon S.S., DesJardin P.E., Presser C., Hewson J.C. & Avedisian C.T., "Numerical modeling and experimental measurements of water spray impact and transport over a cylinder", *International Journal of Multiphase Flow*, **32** (2006), pp. 132–157.