Wind and Structures, Vol. 5, No. 2~4 (2002) 127-140
DOI: http://dx.doi.org/10.12989/was.2002.5.2_4.127

Modelling the capture of spray droplets by barley

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Abstract. This paper presents some of the results of a project whose aim has been to produce a full simulation model which would determine the efficacy of pesticides for use by both farmers and the bio-chemical industry. The work presented here describes how crop architecture can be mathematically modelled and how the mechanics of pesticide droplet capture can be simulated so that if a wind assisted droplet-trajectory model is assumed then droplet deposition patterns on crop surfaces can be predicted. This achievement, when combined with biological response models, will then enable the efficacy of pesticide use to be predicted.

Key words: crop spraying; droplets; crop modelling; canopy flow; deposition patterns.

1. Introduction

There are many factors which a farmer must consider when planning to spray a crop. The first decision is whether spraying is likely to make economic sense; whether the increased yield due to spraying is likely to recoup the costs of the application. The many constraints on spraying must also be considered. A spray application is likely to be very dependant on the local conditions at the time of spraying and these can in turn affect the environmental risk. The drift or other movement of the pesticide off target can cause damage to the natural environment, to other crops or even to people. There are many other considerations such as the risk of resistance forming in the pest population and damage to beneficial flora and fauna. Ideally the farmer should be able to take all of these factors into account and so use the optimum combination of spray composition, nozzle type and timing of application.

This scenario describes the need to create a multi-layer model of spray application to help the

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farmer, and the environment, and which describes the physical and biological processes which determine the pesticide transport, capture and efficacy. The first stage in the construction of such a model network is clearly to be able to define the trajectory of pesticide droplets through the air from the spray nozzle to their location within the plant canopy. This task was undertaken by Mokeba, Salt, Lee and Ford (1997) who modelled the droplets' movement by a Markov trajectory simulation model based upon a calculation of the velocity of a droplet after each of a series of discrete time steps. The velocity of the spray droplets was considered as the weighted sum of their ballistic and random walk components scaled by a factor whose magnitude was determined by the ratio of their velocity components. Account was taken in the model of the effect of crop waving, which dominated the droplet movement within the crop canopy, and a sensitivity analysis was carried out to look at the relative effects of drop size, wind velocity, atmospheric turbulence intensity, evaporation, release height and atmospheric stability parameters.

The next stage in modelling the capture process has been to construct a realistic 3-dimensional parameterisation of the crop, using barley both for its agricultural commonality as well as its relative geometrical simplicity. It is then possible to compare the position and trajectory of the droplet to the positions of plants within the crop to determine when and where the droplet has been captured.

The final stage of this integrated model network is to model the pesticide diffusion and biological control processes arising from known droplet locations on the plant, by which to define to eventual efficacy of the application.

2. Modelling the crop

A simple model of a cereal plant is required to allow the detection of collision between a droplet and the plant without excessive error or computational effort. The parameters of this model should also be as easy to specify as is possible. Fortunately, these two aims are complementary.

Each plant is described by a combination of three types of elements; the stem, any other tillers and, attached to this skeleton, the leaves.

The stem is represented by a vertical cylinder and thus is described by its height and diameter. Additional tillers are likewise approximated by cylinders but these may be attached to the stem at any position and orientation. The additional parameters required are the height of attachment to the stem, the angle of attachment around the stem relative to the x-axis and the angle of the tiller to the vertical.

Each leaf is described by the shape of its main vein, which is assumed to lie in a vertical plane, the width of the leaf at each point along this line and its thickness at each point on this surface as well as the point of attachment of the leaf to the plant.

The shape of the main vein is approximated by a quartic polynomial which defines the height above ground, z, as a function of radial distance, r, from the origin of the leaf (Fig. 1a). This imposes the constraint that the leaf must not curl back on itself.

The width of the leaf is approximated by a constant maximum width in the middle of the leaf with tapering at each end (Fig. 1b). This provides a surprisingly good approximation to a real barley leaf whilst being very simple. However, it would require very little computing effort to specify the width as a function of radius if a suitable model could be found.

The thickness is taken to be constant as small differences probably have little effect. Again, this could be made a function of position on the plane of the leaf for little computing effort.

The point of attachment of a leaf is defined by whether it is attached to the stem or, if not, which

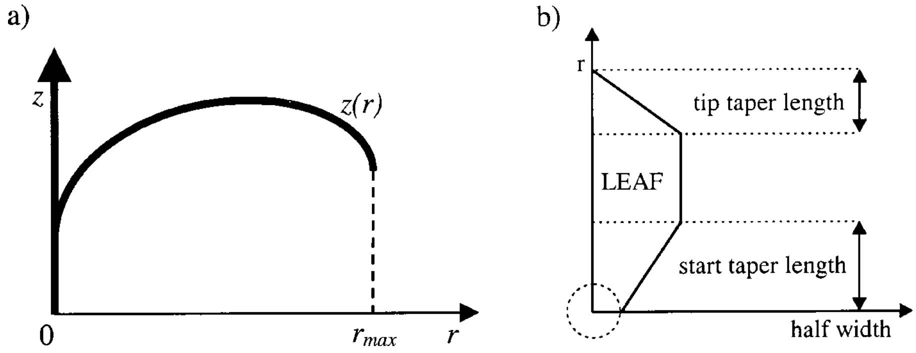

Fig. 1 (a) The main vein as a function of radial distance, (b) The width of the leaf, defined by maximum width and lengths of taper.

tiller it is on. Also vital is the angle of the leaf about this point and this is specified as the angle relative to the x-axis.

To obtain values of the parameters used for the model crop, measurements were made on real barley plants. Due to the time of year, these were grown in a greenhouse in a closely packed array of 20 cm plant pots to simulate conditions in the field as closely as possible. Three photographs were taken of each plant at two and three weeks after planting. One photograph was from directly above and the other two were from the side at an angle of 90° to each other. A ruler was included in each shot for scale.

The plan view photograph allowed direct measurement of the angle about the stem of any tillers and the angles of the leaves about the stem and other tillers. The other two photographs were used to measure the height of the stem, and the heights of tillers and leaves as functions of radial distance from their points of attachment.

Figs. 2a-d show quartics fitted to the data using the method of least squares with the vertical intercept unconstrained except for where it would be negative in which case it is constrained to zero. Observation of these plants and more mature plants in the field supports the assumption that leaves rarely come back on themselves and that therefore the height of their centres can be expressed as functions of radial distance. The least squares regression lines show that quartics provide enough flexibility to adequately approximate these functions.

Barley leaves are often observed to twist. In many cases this twisting appears to be approaching some regular pattern. The radii to cumulative twist angles of $\pi/2$, $3\pi/2$ etc. were measured from the overhead photographs of two week old barley plants. This was done for all leaves except for damaged leaves or those too vertical to measure accurately in this way. For all the barley plants observed, the twisting was anti-clockwise looking along the leaves from base to tip.

An approximation for the cumulative twist angle (CTA) is provided by Eq. (1). In this equation CTA is given in terms of radial distance r from the stem and the distance f to a cumulative twist angle of $\pi/2$.

$$\mathrm{CTA} = \frac{\pi}{2}\frac{\tau^{r/f} - 1}{\tau - 1}, \qquad \tau = 2.2674 \tag{1}$$

The form of this equation was motivated by observing that the angle of the leaf appears to follow a sinusoidal waveform as one moves radially out from the base of the leaf. The period of this

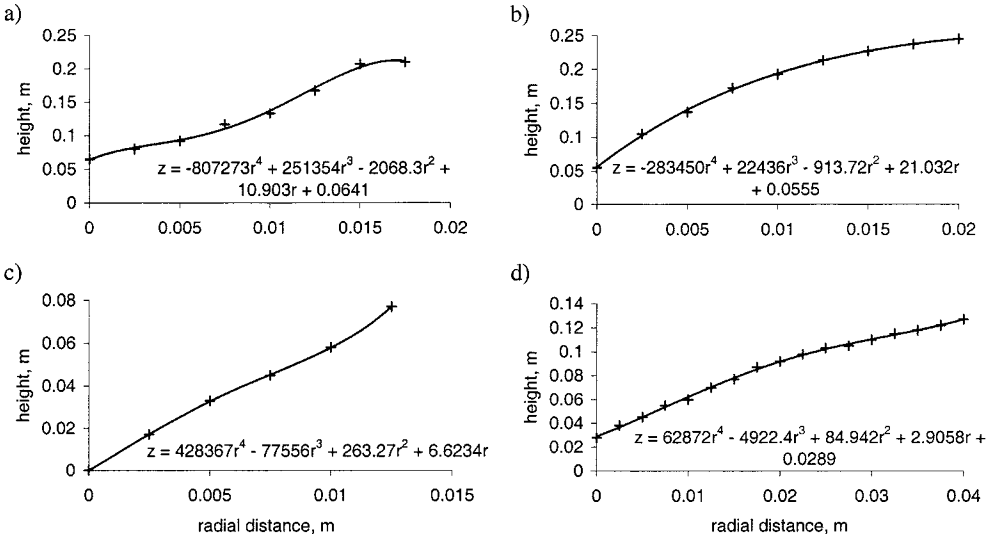

Fig. 2 Approximating the shape of barley leaves a-d by quartics

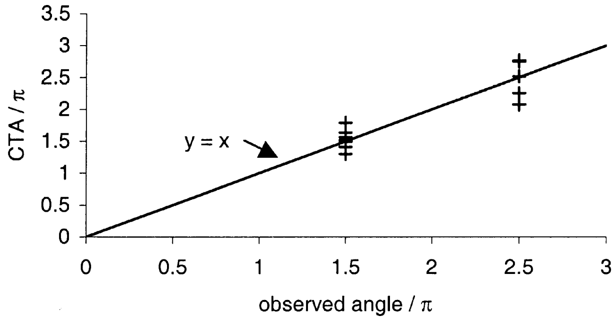

Fig. 3 CTS vs. observed angle for 2 week old barley plants

waveform seems to be uniformly decreasing. τ is the factor this period decreases by every half cycle. The predictions of Eq. (1) versus observed results for two week old plants are plotted in Fig. 3. The parameter τ was chosen to give a regression line of unit gradient when forced through the origin.

Once all the parameters have been specified, the plant may be visualized using the equations within the program. Two such visualizations are illustrated in Fig. 4.

A field of plants may be built up from a number of these individual plants by placing a plant at each position in a grid defined by the row spacing and overall density. For simplicity and ease of analysis a single plant is used. If this plant is typical of the crop then the lack of variety should not have too strong an adverse effect on the results. There will however be a strong pattern to the crop if the orientation of all the plants is the same and this would probably have a marked effect. A rotation is therefore applied to each plant. For simplicity this is defined in a regular fashion on a 10×10 grid of plants by introducing a 36° rotation between each plant along each row and between rows.

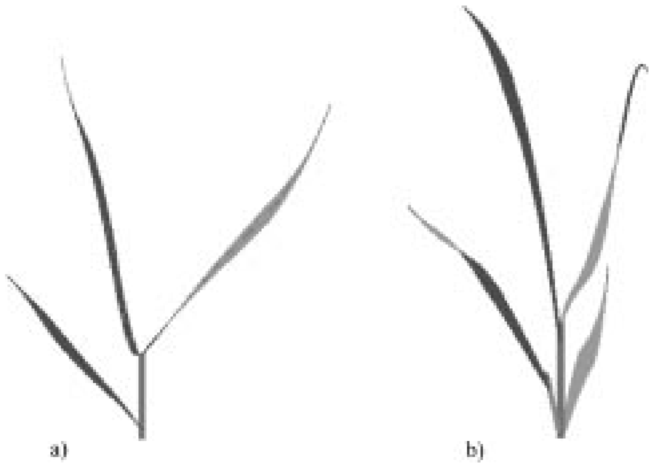

Fig. 4 Computer generated barley plants at (a) 2 weeks and (b) 3 weeks (the lighter shade corresponds to the stem and upper surface of the leaves)

3. Modelling the capture process

3.1. Collision detection

The difficulty of modelling the airflow around individual canopy elements requires that the airflow is averaged as a function of height within the canopy. Account is only made of more local effects once a droplet has come into contact with a canopy element.

Once a droplet enters the canopy there becomes a possibility of it coming into contact with a plant during any time-step Δt. However, it is only feasible to test for contact at discrete points in time. The only times for which position is known are at the end of each time-step. If the droplet is moving too fast then this will create an unacceptably large possibility that the droplet will pass through a plant element without this being detected. To overcome this problem more positions can be tested by linearly interpolating between the positions at the ends of successive time-steps. This is done in such a way that the distance the droplet moves between tests is never more than some specified maximum distance, $\Delta s_{\max}$. An appropriate choice for this distance might be of the order of the thickness of the thinnest leaf.

At each point that is to be tested, it is first determined whether the droplet has come into contact with the nearest stem. Contact must have occurred with the stem if the distance between the centre of the droplet and the centre of the stem is less than the sum of their radii. In fact, contact is only allowed if the centre of the droplet is lower than the height of the stem so that the appropriate distance is the distance in a horizontal plane. The error involved is similar to an error in the height of the stem of about $d/2$; about 0.1 mm compared to a typical stem height of at least 100 mm.

The leaves and any tillers are then taken in turn. For each of these a small circle of plants containing all those for which the element in question could possibly capture the droplet is determined. This is done by realizing that for leaves the centre of the droplet must be within the maximum radius of the leaf from the centre of the stem plus half the maximum thickness of the leaf plus half the drop diameter with the tillers treated similarly.

Considering each of the plants in turn, it is determined whether the particular element has indeed

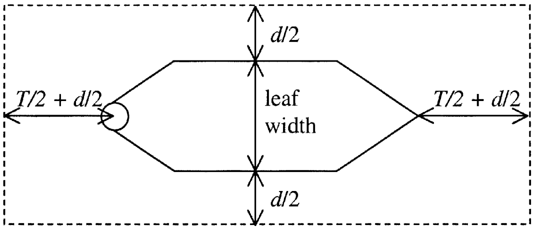

Fig. 5 Bounds of the first proximity test

come into contact with the droplet.

Additional tillers are dealt with similarly to the main stem by considering the minimum distance between the centre of the droplet and the centre of the tiller. However, the end of the tiller is now assumed to be hemispherical in shape.

When considering leaves, the full contact detection routine is preceded by two more approximate tests of the proximity of the droplet to the leaf. This is to save computational effort. The first of these tests is conducted in the *x*-*y* plane by drawing a rectangle around the leaf and only proceeding if the centre of the droplet lies within this area. The rectangle extends a distance equal to half the maximum width of the leaf plus half the droplet diameter each side of the centre of the leaf and half the thickness of the leaf plus half the droplet diameter from each end of the leaf, Fig. 5.

A test is then conducted on the height of the droplet. If a droplet is to contact a leaf then the radial distance in the parameterization of the point of contact on the leaf must lie within $(T+d)/2$ of the radial distance s of the droplet, where T is the thickness of the leaf. The height of the centre line of the leaf at the point of contact must then lie in the range, $z(s) \pm M.(T+d)/2$ where $z(s)$ is the equation of the centre line and M is the maximum gradient of the leaf. The droplet must then lie within an additional $(W+T+d)/2$ of this where W is the maximum width of the leaf. Therefore, bounds on the droplet's height are,

$$z(s) \pm \frac{M.(T+d)+(W+T+d)}{2} \tag{2}$$

Although these bounds are not the strictest possible, they provide a suitable balance between strictness and computational time to make this added test worthwhile. If the droplet lies outside these bounds then it can not be in contact with the leaf and the contact detection routine is stopped.

Once it has been established that the droplet is reasonably close to the leaf, the full, accurate method of detecting contact is used. This involves parameterising the mid-plane of the leaf where the midplane is what the leaf would be with zero thickness. Along the leaf, the radial distance r, from 0 to $r_{\max}$ is used and the position across the leaf is given by a parameter s taking values from -1 to 1 with zero representing the centre line.

The closest point on the surface of the leaf to the droplet is now required. Contact will be considered to have occurred if this distance is less than the radius of the droplet. To achieve this a simplex method of Nelder and Mead (1964) is used to minimize a distance function over the two-dimensional parameter space $\{r, s\}$. The distance function is basically the distance from the droplet's centre to (r, s) on the nearer surface of the leaf. However, the leaf only occupies the region of this space,

$$\{r, s : 0 \leq r \leq r_{\max}, -1 \leq s \leq 1\} \tag{3}$$

The distance function is therefore set to a large value outside this region as a simple method of constraining the algorithm to act only on the limited region of the plane.

The Nelder-Mead algorithm in two-dimensions compares the values of the function to be minimized at each vertex of a triangle and then rejects the vertex with the highest value and replaces it with a new vertex, forming a new triangle. This process continues until the difference between the highest and lowest valued vertices becomes less than some specified tolerance or the maximum number of steps has been exceeded. This limit on the number of steps is required to ensure that the algorithm terminates. For the purposes described here it was decided that a value for the tolerance of 1 μm would provide acceptable accuracy whilst keeping computational time reasonable.

If contact is detected then a better idea of where on the surface this capture occurred is desired. This may differ somewhat from the closest point as found using the Nelder-Mead algorithm due to the distance the droplet travels between checks.

The droplet was in a region of non-contact at the previous test point and is now in a region of contact. It is assumed that there is only one point where non-capture becomes capture on the line between these test points, an assumption implicit in the choice of maximum step size anyway. If it is assumed that the trajectory of the droplet follows the line between these two test points then a bisection method can be used to find the point on the leaf where contact occurred. The number of steps used in the bisection process determines the accuracy and must be considered in conjunction with the maximum distance between checks, $\Delta s_{\max}$.

Once simple collision has been detected by the above methods there are a further two factors to consider before capture can be taken to have occurred. These are a consideration of the local deflection of airflow by the plant element and the possibility of the droplet rebounding from the surface of the plant.

3.2. Local deviations in airflow

The impaction efficiency, E_i can be considered the probability that an individual droplet moving with the air directly towards a suitable capture element will impact. To extend this idea to the desired situation, some account must be made of sedimentation. For, if a droplet is falling under gravity then this component of its motion will not be significantly affected by deflection of the air stream. Thus, if the droplet is moving towards an element of the plant, the corrected probability of collision, P, will be greater than the impaction efficiency alone.

A suitable weighting is required to combine the situations of pure impaction and pure sedimentation. The velocity of the droplet, $\mathbf{v}_{drop}$, may be split into two additive components; the local air velocity, $\mathbf{v}_{wind}$, and the remaining component, $\mathbf{v}_{drop} - \mathbf{v}_{wind}$. The magnitude of these components may be used in a weighting since the magnitude of $\mathbf{v}_{drop} - \mathbf{v}_{wind}$ reflects the importance of sedimentation. The denominator must ensure that P reduces to 1 when $E_i = 1$, as it should. The squares are used since these reflect the relative energies involved in each type of motion and so that in the case where $\mathbf{v}_{drop} - \mathbf{v}_{wind}$ is perpendicular to $\mathbf{v}_{wind}$ the denominator becomes the square of the droplet speed, which is intuitively attractive. The resulting relationship is thus,

$$P = \frac{|\mathbf{v}_{wind}|^2 E_i + |\mathbf{v}_{drop} - \mathbf{v}_{wind}|^2}{|\mathbf{v}_{wind}|^2 + |\mathbf{v}_{drop} - \mathbf{v}_{wind}|^2} \tag{4}$$

The impaction efficiency used is calculated using the approximation of Bache and Johnstone

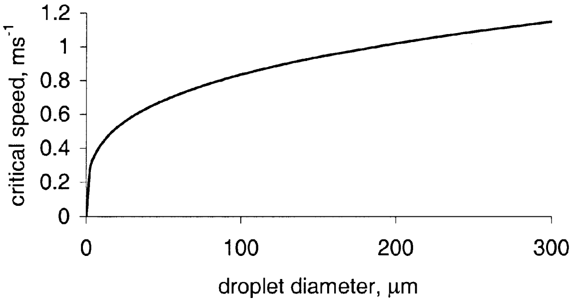

Fig. 6 The variation of u_{crit} with the diameter of droplets for a set of typical parameter values

(1992) to the data of May and Clifford (1967). The velocity used to calculate the Stokes number is taken to be $\mathbf{v}_{wind}$ since this is the velocity used to weight impaction. In line with May and Clifford (1967), the characteristic length used for the Stokes law is the width of the leaf at the point of contact perpendicular to $\mathbf{v}_{wind}$, that is the width the wind sees. If $\mathbf{w}_{leaf}$ is the vector across the width of the leaf at the point of contact then the characteristic length,

$$l = |\mathbf{w}_{leaf}| - \frac{\mathbf{v}_{wind} \cdot \mathbf{w}_{leaf}}{|\mathbf{v}_{wind}|} \tag{5}$$

3.3. Rebound model

To construct a model of rebound the critical velocity concept of Lake and Marchant (1983) is used where a droplet will rebound if and only if its speed is greater than some critical speed u_{crit}. Although their experiment was only conducted over a limited range of values, the compositions of the droplets were appropriate to pesticide spraying and the leaves used were barley so the results should be applicable. The leaf surface parameter, λ, is interpreted as characterizing the roughness and waxiness of the leaf surface and is therefore held constant at 381 µm as used by Lake and Marchant. Unfortunately, the smallest droplets they used had a diameter of 80 µm so particular care must be taken if applying their results to smaller droplets, particularly those smaller than about 20 µm, Fig. 6.

In the case of rebound, the trajectory of the droplet is taken to be reflected by the tangential plane to the leaf at the point of contact. The droplet loses kinetic energy in the process of rebounding. If the droplet has incident speed v_0 and rebounds with speed v_1 then the idea that, in the limit as v_0 becomes large there appears to be a constant coefficient of restitution e, leads to the relationship,

$$v_1 = e(v_0 - u_{crit}) \tag{6}$$

Hartley and Brunskill (1958) found a value for e of 0.6 for water droplets. Webb *et al.* (2000) made measurements of v_0, v_1 and u_{crit} for 12 droplets of varying size and composition. The values of e calculated from this data ranged from .42 to .83. A least squares regression forced through the origin gave a value of 0.59 for e with Eq. (6) seeming to provide a good fit to the data.

4. Results and discussion

4.1. Validation

Measurements in well documented, controlled conditions have been made by (Hislop *et al*. 1993) who sprayed young barley plants in a spray chamber *cum* wind tunnel with a variety of nozzle types. Their primary aim was to investigate the effects of air assistance. Despite this, half the results are with no air assistance and so are useful for comparison here.

The plants used were 170 mm tall barley plants grown outdoors with 4 leaves on the main tillers. The plants chosen for the modelling in section 2 were 250 mm tall at the 4 leaf stage but it was decided to use these plants, Fig. 4(b), rather than the plants of the correct height which only had three leaves, Fig. 4(a). This was because the orientation and structure of the leaves is probably more important than the overall density. The row-spacing and stem density were set to that described by Hislop *et al*.

The spray solution was sprayed from a boom consisting of three nozzles 50 cm apart. Spraying was conducted at three boom speeds; 0.5, 1.0 and 2.0 ms^{-1}. The nozzles were oriented with the fans perpendicular to the crop rows and three different angles were used for the nozzles; 45 degrees forwards, 45 degrees backwards and vertical. In each case the nozzles were maintained at 40 cm above the top of crop. The two types of nozzle used in the experiment were characteristic of very fine / fine (VF/F) and medium (M) spray qualities respectively under the BCPC International Spray Classification Scheme .

The situation described above was replicated in the simulation, using 4000 droplets for each run. Since Hislop *et al*. only looked at results of the centremost plants, the results here are limited to capture within a 2 metre square of the nozzle, to simulate this. This aspect of the experimental set up of Hislop *et al*. means that the effect of many of the smaller droplets moving some distance from the nozzle but still reaching the crop is neglected.

The major indicator studied by Hislop *et al*. was the volume of spray captured on the plants. They drew a number of conclusions from their results, some of which are applicable to the non air-assisted case and are therefore suitable to compare with the results of the simulation carried out here. Rather than directly comparing spray volumes, which will differ simply because of differences in the plants used, it is the percentage of spray not drifting caught on the plant which is used to investigate the effects of varying the parameters in the same way as Hislop *et al*.

Hislop *et al*. observed that spraying vertically downwards deposited considerably lower volumes on the crop than both forwards ($+45^{o}$) and backwards (-45^{o}) angling for both nozzle types examined. Angling the nozzles forwards produced greater deposits than when they were angled backwards. This effect, that angling the nozzles increased the level of deposits is also found with the simulation, Fig. 7. However, angling the nozzle forwards in the simulation produced slightly smaller deposits than angling it backwards.

Secondly, Hislop *et al*. found that, for all trajectories, the finer nozzle (VF/F) produced greater volumes on the crop than the coarser nozzle (M). The same result is produced by the simulation, Fig. 8, though the difference between the nozzles is larger than that found by Hislop *et al*. This may be due to the larger number of small droplets produced by the finer quality nozzle which may drift too far to be captured on the plants analyzed by Hislop *et al*.

Overall, the simulated results have reproduced some of the important features of the experimental results of Hislop *et al.* (1993). The difference between the nozzles is very clear as is the interesting

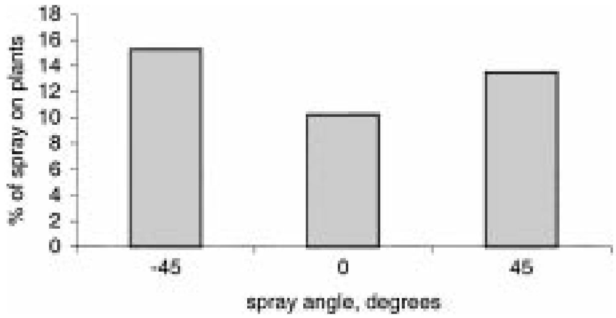

Fig. 7 Simulation results. The effect of spray angle on the volume of plant deposits

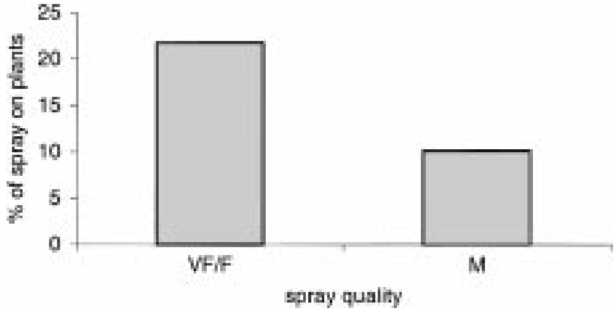

Fig. 8 Simulation results. The effect of spray quality on the volume of plant deposits

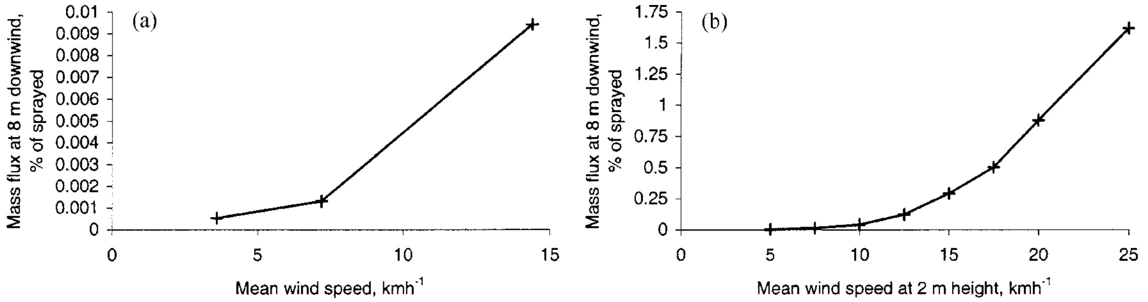

Fig. 9 The relationship between drift and wind speed (a) recorded by Hislop *et al*. (1993), (b) found using the simulation model

effect of angling the nozzles.

Hislop *et al*. (1993) also measured the proportion by volume of sprayed material which was drifting 8 m downwind of their boom though now with a 460 mm tall crop. Fig. 9(a) shows their results for vertical very fine / fine quality nozzles without air assistance. The model simulation used a barley crop of the same height and density and produced the results of Fig. 9(b), where the non-linear nature of the relationship appears to agree well with the experimental results of Hislop *et al*.

4.2. Simulation model capabilities

The influence of a large number of parametric variations can be investigated using this simulation model. Whilst space does not permit a full range of the model's capablities to be demonstrated some significant features will be indicated here.

A major factor in crop spraying, which is easily manipulated, is the choice of nozzle. The data contained in Table 1 allows 4 sizes of hydraulic flat-fan nozzle to be compared. Whilst each nozzle produces some droplets of all sizes, the shift of the droplet spectrum towards larger droplets with larger nozzle is clear. Fig. 10 demonstrates the increased drift with larger nozzles.

The choice of nozzle does not affect just the position of capture, it also affects the volume of spray which is caught by the crop rather than falling to the surface of the soil. Fig. 11 shows a decrease in capture, and thus an increase in canopy penetration, with increasing nozzle size. Fig. 12 shows very low capture of large droplets over 250 um as well as the smallest droplets of below 50 μm

Table 1 Nozzle size information

Size code	Quality	% < 100 μm	% > 350 μm	V.M.D.
01	Very fine / fine	21.03	2.15	150.77
02	Fine	13.37	8.18	191.79
04	Medium	6.35	22.73	263.88
08	Coarse	3.56	50.56	355.12

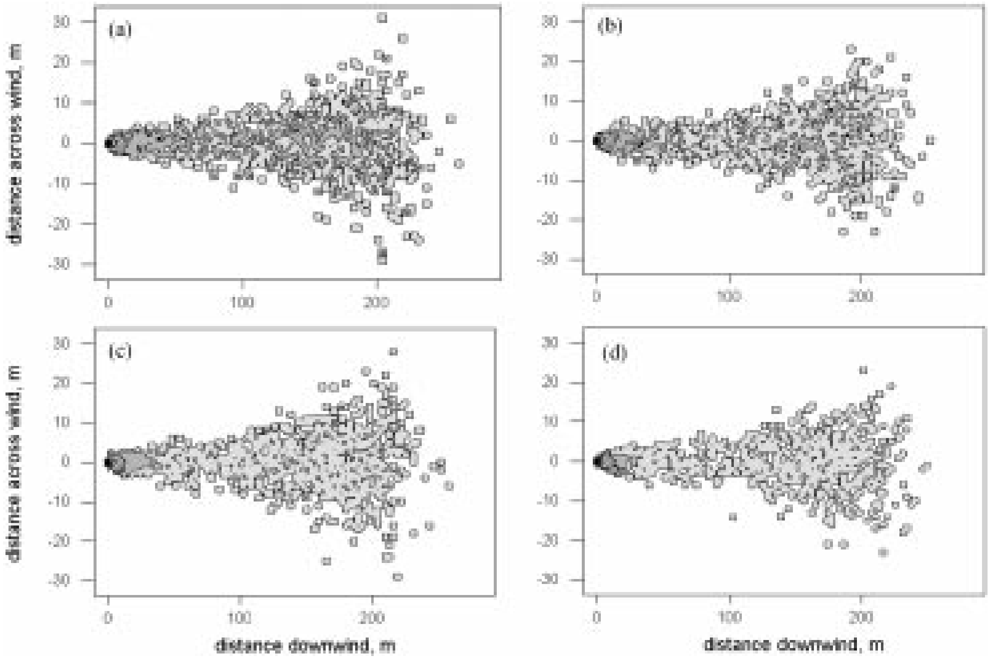

Fig. 10 The deposition patterns from 4 nozzles with size codes (a) 01, (b) 02, (c) 04, (d) 08 (Logarithmic scale with each division representing a factor of 100 in the area density of the deposited volume. Darker shading corresponds to greater density)

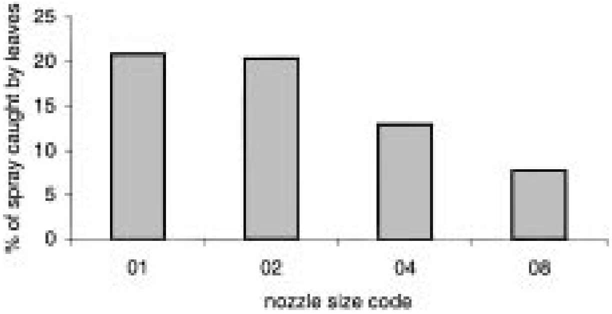

Fig. 11 The effect of nozzle size on the volume of spray caught by the leaves of the crop

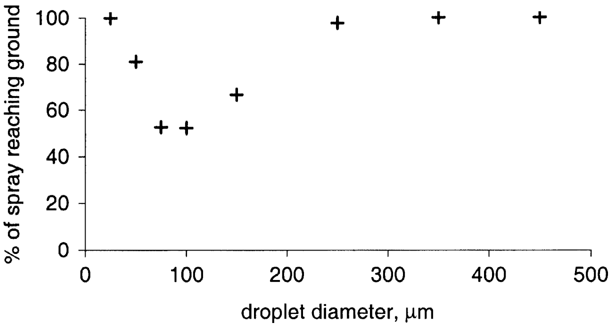

Fig. 12 The effect of droplet size on the volume of spray caught by the leaves of the crop

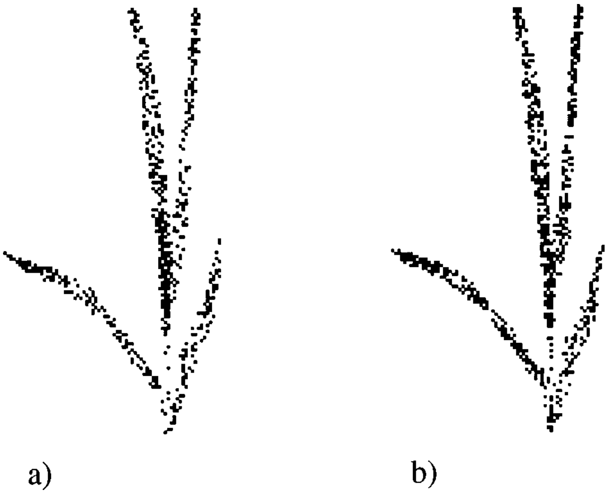

Fig. 13 The pattern of deposits on the leaves of an individual plant for 2 nozzles (a) size 01, (b) size 08

though these small droplets will have little effect on the total volume deposited. The differences between droplets of different sizes may be attributable to the different trajectories of different sized droplets as well as the influence of size on the capture process nearer the leaf surface.

As might be expected, given the high penetration of the canopy, the distribution of deposits is fairly even over individual plants for all the nozzles considered, Fig. 13. It is also possible to make out from Fig. 13 the slightly higher number of deposits given by the 08 nozzle compared to the 01 nozzle.

4.3. Nozzle choice

Suppose a decision as to which nozzle to use were to be made based upon these results. It can be seen that a larger nozzle reduces any drift problem and produces more deposits, both of which are usually desirable. However, it will also produce lower volumes on the crop and more on the soil which is undesirable. Therefore, the farmer must yet again balance a number of conflicting issues with the optimal decision probably being sensitive to the precise conditions in the field. Modelling can still play a vital role, however, by alerting the farmer to the most pertinent variables and suggesting an idea of the best solution to any particular spraying problem.

It is obvious that increasing the spray sheet speed will reduce drift, Fig. 14, by forcing droplets lower. Not quite so obvious is the effect that the higher droplet speeds within the crop will have on capture. A droplet is more likely to exceed the critical speed for rebound the faster it is travelling. Therefore, a higher spray sheet speed corresponds to more rebound and so greater penetration of the crop and less capture by the leaves, Fig. 15. This must outweigh the other effect of increased impaction efficiency at higher speeds which would, by itself, increase the volume of spray caught by the crop.

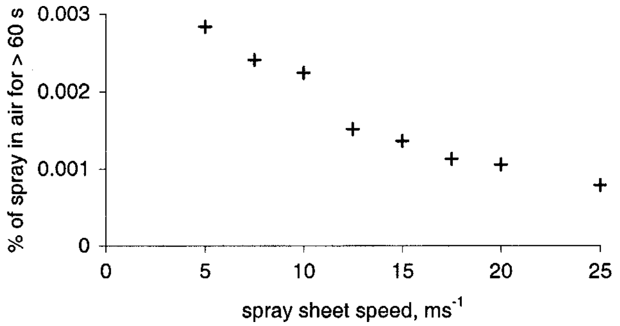

Fig. 14 The decrease in drift with increasing spray sheet speed

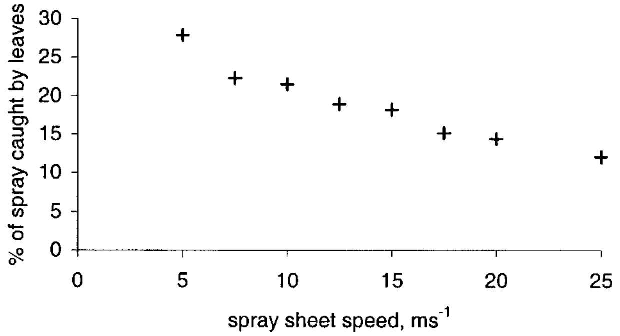

Fig. 15 The decrease in spray capture with increasing spray sheet speed

5. Conclusions

The first aim of the project from which this paper has been derived has been to develop a model for the capture of spray droplets using a realistically modelled crop. The paper demonstrates how the crop model was developed and how the droplet capture mechanisms have been simulated together with the most important effects of some of the parameters of the model. The ability of the model to allow the effects of many different parameters to be investigated by recording the corresponding responses is the main conclusion to be drawn from this analysis.

The visualization of the deposits on single plants, Fig. 13, demonstrates the potential of this type of approach most distinctly.

One possible output from this model is the density and sizes of deposits on a leaf surface. A model of biological response for leaf diffusion and fungal growth with the potential to utilise this droplet transport information has been developed, Cox, Salt, Ford, Chowdhury and Lee (2000), which shows promise in comparison with experimental results of the germination and initial growth stages of *E. graminis*.

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