Dorr, Gary J., Kempthorne, Daryl, Mayo, Lisa C., Forster, W. Alison, Zabkiewicz, Jerzy A., McCue, Scott W., Belward, John A., Turner, Ian W., & Hanan, Jim
(2014)
Towards a model of spray-canopy interactions : interception, shatter, bounce and retention of droplets on horizontal leaves.
Ecological Modelling, *290*, pp. 94-101.

Towards a model of spray-canopy interactions: interception, shatter, bounce and retention of droplets on horizontal leaves.

Gary J Dorr [a,e], Daryl Kempthorne [b], Lisa C Mayo [b], W Alison Forster [c], Jerzy A Zabkiewicz [d], Scott W McCue [b], John A Belward [b], Ian W Turner[b], Jim Hanan [a]

[a] The University of Queensland, Queensland Alliance for Agriculture and Food Innovation, Biological Information Technology, Brisbane, Australia
[b] Mathematical Sciences School, Queensland University of Technology, Brisbane, Australia
[c] Plant Protection Chemistry NZ Ltd, Rotorua, New Zealand
[d] SciCon Scientific Consultants, Rotorua, New Zealand.
[e] Corresponding Author,
Email: g.dorr@uq.edu.au, Phone: +61754601350, Mobile: +61401148192
Address: The University of Queensland, Gatton, QLD 4343, Australia

Abstract

Pesticides used in agricultural systems must be applied in economically viable and environmentally sensitive ways, and this often requires expensive field trials on spray deposition and retention by plant foliage. Computational models to describe whether a spray droplet sticks (adheres), bounces or shatters on impact, and if any rebounding parent or shatter daughter droplets are recaptured, would provide an estimate of spray retention and thereby act as a useful guide prior to any field trials.

Parameter-driven interactive software has been implemented to enable the end-user to study and visualise droplet interception and impaction on a single, horizontal leaf. Living chenopodium, wheat and cotton leaves have been scanned to capture the surface topography and realistic virtual leaf surface models have been generated. Individual leaf models have then been subjected to virtual spray droplets and predictions made of droplet interception with the virtual plant leaf. Thereafter, the impaction behaviour of the droplets and the subsequent behaviour of any daughter droplets, up until re-capture, are simulated to give the predicted total spray retention by the leaf. A series of critical thresholds for the stick, bounce, and shatter elements in the impaction process have been developed for different combinations of formulation, droplet size and velocity, and leaf surface characteristics to provide this output.

The results show that droplet properties, spray formulations and leaf surface characteristics all influence the predicted amount of spray retained on a horizontal leaf surface. Overall the predicted spray retention increases as formulation surface tension, static contact angle, droplet size and velocity decreases. Predicted retention on cotton is much higher than on chenopodium. The average predicted retention on a single horizontal leaf across all droplet size, velocity and formulations scenarios tested, is 18, 30 and 85% for chenopodium, wheat and cotton, respectively.

Keywords
Agrichemical spray, mathematical model, pesticide application, spray retention, droplet impaction, leaf surface model

1 Introduction

The challenges facing agrichemical users have increased in complexity over recent years. On the one hand, consumers require the highest quality of produce, while on the other, regulators insist on safety (to the consumer from residues) and risk reduction (to the operator, environment or ecosystem) (Zabkiewicz, 2007). The requirement to reduce detrimental ecological effects and retain or improve both biological efficacy and the economic viability of the grower can only be met by optimising spray efficacy through smarter and more cost effective spray formulation and application. These factors must be considered together as they are linked inextricably (Zabkiewicz, 2007) if optimal canopy penetration and coverage is the objective.

Many spray programmes currently employed in the agricultural industry appear to provide lesser control of pests than might be expected from laboratory trials, which can be attributed to inadequate canopy penetration and foliar coverage. Spray adjuvants and the correct choice and use of spray application equipment are powerful tools to maximise pesticide efficacy, reduce detrimental environmental effects and improve the economic viability of the grower.

Expensive field measurements of specific crop/environment combinations are currently required to determine optimal adjuvant formulations and spray application technology. The use of mathematical and computational models to help predict such behaviours could provide a more cost effective alternative, provided they can reliably predict total plant retention, within-canopy distribution, leaf coverage or spray solution run-off.

Previous studies have resulted in empirical models for initial adhesion (Forster et al., 2005) and spray retention (Forster et al., 2006; Pathan et al., 2009) by individual plants. These models utilise parameters that describe solution properties, spray droplet physical properties and leaf surface characteristics. Further progress has been made on various elements of the spray retention process. However, there is a need for a coherent overarching simulation package that is based on process-driven principles instead of empirical chemical-crop environment specific scenarios.

Models for spray deposition from aerial application do exist (Teske et al., 2002), however the focus has been on spray drift, not retention. Models of spray deposition through the plant canopy (Dorr et al., 2008), or impaction onto the plant (Bergeron et al., 1999) also exist. However, these models make the simplifying assumption that if a plant intercepts a droplet, it is always retained. Process-driven models for retention, taking into account droplet bounce and shatter, have recently been implemented within AGDISP (Schou et al., 2012). The focus of the current paper is on further developing process-driven models for droplet interactions with the plant, at or after interception. The innovation of the system presented here is that virtual leaf surface models have been developed and then subjected to virtual spray droplets, with predictions made of droplet interception and retention by the plant leaves. The model inputs include formulation, droplet and plant parameters, so the model will be able to help pick the best formulation and droplet size spectrum to be used for a given plant/crop. These inputs will need to be modified by intelligent operational choices to avoid excessive spray drift while maximising retention in reality.

The construction of a virtual surface with which the droplets may interact is, in itself, a challenging problem. In order to capture a large, accurate data set the technology of scanners and their operation requires a significant amount of experience. Work reported by Loch

(2004), investigated the use of piecewise cubic elements to interpolate a point cloud by a surface with a continuous gradient. In that work the use of a hand held scanner was addressed and an initial investigation of pathways of surface droplets under gravity was made. A theoretical analysis of the interpolation technique was made by Turner et al. (2010) and Oqielat et al. (2011) investigated two techniques for derivative estimation. In this paper a quasi one dimensional model of the movement of a droplet, incorporating gravity and some surface effects was presented. Experiments with were made by putting water droplets onto a leaf and recording their paths. In Kempthorne et al. (2012) and Kempthorne et al. (2013) least squares approximation of point clouds by linear combinations of smooth splines was investigated. These were the surface fitting techniques used in the current work for which efficient numerical linear algebra algorithms have been constructed.

This paper reports on the development of process-based models for adhesion and retention, using a simplifying assumption of horizontal surfaces and droplets impacting perpendicular to the surface. The model is then tested for three different formulations on three plant leaf examples with differing surface shapes and impaction characteristics.

2 Model Description

2.1 Overview

Mathematical models of droplet impaction processes at multiple scales are being developed and integrated to help quantify, optimise and predict the complexities of agrichemical spray retention by plants. Parameter-driven interactive software has been implemented to enable the end-user to study and visualise a variety of practical agrichemical scenarios. Actual plant leaves have been scanned to capture the surface topography and a realistic virtual leaf surface model generated as an integral component of a structural model of an entire virtual plant. Virtual spray droplets are then applied to the leaf model and predictions made of droplet interception and retention by the plant leaf.

2.2 Leaf surface models to provide virtual reproductions of leaf topography

A leaf surface representation was generated to act as the target for the droplet interception and impaction models. To generate these surface representations a large number of three-dimensional data points were captured from an actual leaf surface. Cotton and chenopodium leaves were scanned using an Artec S™, by Artec Group (www.artec3d.com), which is a 3D white light scanner. This scanning process produced a cloud of data points, which was then used as an input for a surface fitting algorithm (Kempthorne et al., 2013; Oqielat et al., 2011). This technique provides the ability to control the coarseness of the underlying mesh, with coarser meshes providing shorter simulation times for the spray droplet trajectory model. The surface is constructed using D^2-splines (Arcange et al., 2004), which minimises a combination of the squared residuals between the fitted surface and the collected data and the curvature of the surface.

This process is displayed for a chenopodium leaf in Figure 1. A photograph of the scanned leaf is shown in Figure 1(a). The point cloud of the scanned leaf contained 105,846 data points and is shown in Figure 1(b). This dataset was then used to generate a mesh of 6,921 points and 13,226 triangles, displayed in Figure 1(c). The resultant surface is shown in Figure 1(d), where the photograph in Figure 1(a) has been texture mapped onto the surface. The surface can be presented in a format suitable for use with the spray droplet trajectory model described in the following section.

2.3 Modelling spray droplet trajectories and interception by leaves on virtual plants

L-studio, a Windows-based software environment for creating simulation models of plants (Prusinkiewicz, 2004; Prusinkiewicz et al., 2007), was used in this study. The leaf surfaces from section 2.2.1 were imported into the 'cpfg' (plant and fractal generator with continuous parameters) component of L-studio using the Tsurface specification (Mech, 2005). L-system based models of the whole plants can be extended to incorporate the detailed leaf surface models and the spray interception model. A particle trajectory model that uses a combined ballistic and random walk approach, as described by Dorr et al. (2008), was used to model the movement of spray droplets through the air. It calculates the trajectory of the droplets from release to final impact and determines if they impact on any leaf; if so, their incidence angle and velocity is determined at impaction. Any droplets that are released through shatter or bounce are tracked until all droplets are accounted for, including those lost to the ground or that drift away from the sprayed area. A complementary output is the distribution of spray throughout the canopy. The single plant outputs can be also amalgamated into a multi-plant (same or different species) model to simulate spray retention by entire crops or crop/weed populations.

2.4 Spray droplet impaction models to calculate adhesion, bounce or shatter behaviour

When a droplet impacts on a leaf surface, there are three possible outcomes, namely adhesion, bounce or shatter. The model by Mao et al. (1997) is used to describe the droplet's interaction with the leaf surface, leading to either adhesion or bounce. Their model considers only a horizontal surface (Sikalo et al., 2005) and does not apply if the droplet shatters on impact. Modelling of the shatter process is at a less advanced stage than spread and bounce (Mercer et al., 2007; Mundo et al., 1995; Mundo et al., 1997; Yoon and DesJardin, 2006; Yoon et al., 2006). Key physical parameters included in these models are the properties of the formulation (dynamic viscosity, surface tension and density) and droplet physical properties (diameter and downward velocity).

2.4.1 Modelling droplet bounce

Droplet spread and rebound is typically modelled by balancing changes in the kinetic and surface energy of a droplet once it has impacted a substrate. Attané et al. (2007) presented a one-dimensional energy balance model describing the spreading and recoiling motions of a droplet impacting a horizontal surface, which was then extended by Mercer at al. (2010) to produce a predictor for bounce. This model, however, requires the solution of a second order nonlinear ordinary differential equation for each droplet impaction which can become time consuming. An alternative model, by Mao et al. (1997), was instead favoured for its use of purely algebraic equations as well as its better agreement with (unpublished) experimental data.

By comparing energy states of the droplet at key stages of the impact process, the energy balance model presented by Mao et al. (1997) predicts the maximum spread diameter of the droplet after impact, and its tendency to bounce after subsequent recoil. The model enforces conservation of volume throughout the impaction process and assumes that the droplet shape at maximum spread can be approximated by a thin cylindrical disk.

Maximum spread diameter, d_{m}, is predicted by equating the system energy before impaction (consisting of surface and kinetic energy) to that at the moment of maximum spread (consisting of surface energy and accounting for kinetic energy lost due to viscous dissipation in the spreading process). To calculate d_{m}, the cubic equation

$$\left[\frac{1}{4}(1-\cos\theta_{\mathrm{e}})+0.2\frac{\mathrm{We}^{0.83}}{\mathrm{Re}^{0.33}}\right]\left(\frac{d_{\mathrm{m}}}{D}\right)^3-\left(\frac{\mathrm{We}}{12}+1\right)\left(\frac{d_{\mathrm{m}}}{D}\right)+\frac{2}{3}=0$$

from equation (17) of Mao et al. (1997) must be solved. This equation incorporates the system parameters through the Weber number $\mathrm{We}=\rho V^2 D/\sigma$, the Reynolds number $\mathrm{Re}=\rho V D/\mu$, and the equilibrium (static) contact angle θ_{e}. Note that V and D are the impact velocity and initial diameter of the droplet respectively, ρ is the fluid density, σ is the surface tension at the fluid-air interface, and μ is the fluid viscosity. The above cubic equation can be solved exactly for d_{m}; if we write the polynomial in its monic form, $x^3+px+q=0$, then the real root is given by

$$\frac{d_{\mathrm{m}}}{D}=\left[-\frac{q}{2}+\sqrt{\left(\frac{q}{2}\right)^2+\left(\frac{p}{3}\right)^3}\right]^{1/3}+\left[-\frac{q}{2}-\sqrt{\left(\frac{q}{2}\right)^2+\left(\frac{p}{3}\right)^3}\right]^{1/3}.$$

In order to use this result, the inequality

$$\left(\frac{q}{2}\right)^2+\left(\frac{p}{3}\right)^3<0$$

must be checked first. If this condition is not met, then no real solution for d_{m} exists. Fortunately this only occurs for relatively small initial droplet diameter D and impact velocity V, where it is likely that the droplet adheres to the surface and calculation of d_{m} is not required.

Bounce is predicted by determining whether the recoil stage after maximum spread will provide enough kinetic energy to the droplet to allow it to re-form into a spheroid and lift off the surface as a whole. If the energy is not available for rebound, the droplet will adhere to the surface. Mao et al. (1997) predict bounce through the equation

$$E_{\mathrm{ERE}}=\frac{1}{4}\left(\frac{d_{\mathrm{m}}}{D}\right)^2(1-\cos\theta_{\mathrm{e}})-0.12\left(\frac{d_{\mathrm{m}}}{D}\right)^{2.3}(1-\cos\theta_{\mathrm{e}})^{0.63}+\frac{2}{3}\left(\frac{D}{d_{\mathrm{m}}}\right)-1\,.$$

This equation specifically determines the 'excess rebound energy' (E_{ERE}) of the droplet as a function of the maximum spread diameter d_{m}. A value of E_{ERE} greater than zero indicates sufficient energy for bounce and a zero or negative value indicates adherence. This leads to an extension of the Mao et al. (1997) model, where a positive nonzero E_{ERE} can be used in the calculation of the exit velocity of a bouncing droplet through the relation

$$V_{\mathrm{exit}}=\sqrt{\frac{12E_{\mathrm{ERE}}}{\pi\rho D^3}}.$$

In the present study, the direction that the droplet bounces is assumed to be a mirror of its incoming direction. This simplifying assumption makes most sense when the impaction occurs perpendicularly onto a horizontal surface, since the droplet would be expected to rebound upwards (at least in the absence of surface defects). For impactions involving angled surfaces or trajectories, the concept becomes more complex, with factors such as energy loss playing a role in determining the precise path of the bouncing droplet. These complexities are not considered by the simplified mirror assumption, and are the subject of further work.

Additionally, a 'bounce boundary' may be generated for each spray formulation and plant type combination by running the Mao model as described above for a range of initial droplet diameters D and impact velocities V. When plotted on V and D axes, the points where E_{ERE} switches from negative to positive connect to form a curve that delineates the border between bounce and adhere results.

2.4.2 Modelling droplet shatter

Due to droplet shatter being less well understood than spread and bounce, the bulk of the literature relies on empirical relations to predict the onset of shattering. A sound theoretical argument can be made that droplet shatter occurs when the inertial forces from impact overcome the capillary effects of the fluid. A relation can be written in terms of the Weber and Reynolds numbers but must be empirically fitted to data (Moreira et al., 2010). Mundo et al. (1997) use one such relation, $K = \mathrm{We}^{1/2}\mathrm{Re}^{1/4}$. They found that a critical value of K, $K_{\mathrm{crit}} = 57.7$, correlated well to the shatter boundary for their data. The value K_{crit} delineates shatter results from non-shatter results: if the calculated K on impact is greater than K_{crit} then the droplet will shatter, otherwise it will either bounce or adhere.

Laborious adhesion and shatter experiments would normally be required to empirically fit a suitable value of K_{crit} to a new data set, which is counterproductive to the modelling objective. Forster et al. (2010), however, devised a simple method to overcome this issue by providing an estimation of K_{crit} based on two contact angle measurements of standardised formulations. This approach is used here to calculate K_{crit} for each plant type, and shatter is predicted if the computed value of Mundo et al.'s criterion exceeds this.

The shatter criterion has the shortcoming that it does not give any information about the satellite droplets formed in the shatter event; it merely acts as an indicator of whether splash occurs or not. Yoon & DesJardin (2006) present energy balance arguments to account for the distribution of energy to the satellite droplets after shatter. They also summarise linear stability theories that may be used to predict the number of satellite droplets formed on impact, N_s. We take their equation (21) (originally presented in Marmanis and Thoroddsen (1996)),

$$N_{\mathrm{s}} = 0.1\,\mathrm{Re}_1, \quad \mathrm{Re}_1 = \frac{V}{2\sqrt{\mu/\rho}}\left(\frac{\pi^2\rho D^3}{\sigma}\right)^{1/4},$$

to predict the number of satellite droplets, and use conservation of volume (between pre-impact and post-splash states) to predict the diameter of each as $D_{\mathrm{sat}} = D/N_{\mathrm{s}}^{1/3}$.

To calculate the exit velocity of each satellite droplet, Yoon & DesJardin (2006) form energy balance arguments much like those in Mao et al. (1997), leading to

$$E_{\mathrm{KE}} = \frac{\pi}{4N_{\mathrm{s}}} d_{\mathrm{m}}^2(1 - \cos\theta_{\mathrm{e}})\sigma - \pi\sigma D_{\mathrm{sat}}^2\,,$$

for the kinetic energy of each satellite droplet, E_{KE}. We then use the following equation to calculate the exit velocity of each droplet:

$$V_{\mathrm{exit}} = \sqrt{\frac{12E_{\mathrm{KE}}}{\pi\rho D_{\mathrm{sat}}^3}}.$$

The values for E_{KE} can become negative for certain parameters (in particular for low contact angles and when the number of satellite drops becomes large) and hence no real solution for

V_{exit} exists. Even situations where E_{KE} is positive but very close to zero may pose a problem in practice, because V_{exit} will in turn be so small that the satellite droplets will not actually splash away from the site of impaction. To overcome this limitation we include the condition that if E_{KE} is calculated to be less than $\pi\rho V^2 D_{\mathrm{sat}}^3/1200$, we set $E_{\mathrm{KE}} = \pi\rho V^2 D_{\mathrm{sat}}^3/1200$. This ensures that V_{exit} may never be less than $0.1V$, a value which we consider an appropriate lower bound on the exit velocity to ensure that satellite droplets will splash away.

The angle of ejection for each satellite droplet is taken from Dorr (2009), based on empirical random distributions of mean and variance.

3 Model Evaluation

By combining leaf models (section 2.2) with droplet trajectory (spray) models around plants (section 2.3) and impact models (section 2.4) it is possible to provide realistic simulations of spray retention based on real plants and formulations. Leaves of varying size and character were chosen to provide diverse target types. Similarly, representative formulations with specific physicochemical properties were used to provide a range of input parameters. The outputs from the models described above can be tested against laboratory data for individual leaf retention (involving droplet adhesion and secondary capture from bouncing or shattered droplets) to validate the accuracy of the overall single leaf retention model.

3.1 Single leaf

The model described in section 2.2 was run for various droplet sizes, droplet velocities, leaf types and spray mixtures. Droplet size ranged from 100 to 700 µm in 100 µm increments. Droplet velocities were selected to be 1, 3, 6 and 9 m/s. A regular grid of mono-sized droplets at 1 mm spacing was generated and allowed to fall vertically so that the whole leaf surface was covered (Figure 2).

Three leaf types were tested: cotton, wheat and chenopodium. Cotton leaves are easy to wet, whereas chenopodium and wheat leaves can be described as difficult to wet. Wheat provides an example of a grass plant while cotton and chenopodium are broad leaf plants. The leaves were modelled as described in section 2.2.1. Cotton was tested with a coarse mesh consisting of 70 triangles and a calculated area of 2848 mm². Due to the long, thin and curved nature of the wheat leaf, a mesh consisting of 2271 triangles was used with a leaf area of 1848 mm². The output of the chenopodium leaf model was saved at two levels of detail. Initial testing was with a coarse mesh that consists of 100 triangles for the leaf and these results were then compared to a fine mesh that contains 13,266 triangles per leaf at a 3m/s droplet impact velocity. The calculated area of the chenopodium leaf was 731 mm² for the coarse mesh and 736 mm² for the fine mesh. The main reason for the difference in area for the two mesh details is due to edge effects, since the finer the mesh improves the approximation of the leaf edge.

Three spray mixtures were selected to simulate our models: water only, 0.1% Ecoteric® T20 (Huntsman) and 0.1% Pulse® (Nufarm Ltd). The physical properties used for model inputs are shown in Table 1. In order to estimate these properties, the following approaches were employed. Surface tension was measured using a Krüss bubble pressure tensiometer (BP 2 MKII). Static contact angles of each formulation were measured using a KSV CAM 200 optical contact angle meter with a Basler digital video camera. Finally, K_{crit} was estimated according to Forster *et al.* (2010) from static contact angles of 20% and/or 50% aqueous acetone solutions on each leaf surface.

4 Results

The predicted retention of the spray on each of the three leaf types with different spray mixtures, droplet sizes and droplet velocities are shown in Tables 2 to 4. The retention is expressed as a percentage of the total volume of spray droplets that impact the leaf. Unshaded cells indicted that the primary droplets adhere on impact. The lightly shaded cells indicate that the primary droplets bounce on impact and the total retention values shown are due to subsequent recapture of the bouncing droplets. The dark shaded cells indicate that the primary droplets shatter on impact and the total retention values shown are due to the recapture of the daughter droplets.

A comparison of a fine chenopodium leaf surface mesh and a coarse mesh on spray retention is shown in Table 5. Spray retention obtained from the fine mesh was slightly higher than obtained from the coarse mesh, although the same trends in the results were observed.

5 Discussion

5.1 Droplet size and velocity of impacting drops

Predicted retention of the spray on all three single leaves tended to decrease with increasing droplet size and increasing droplet velocity of impacting droplets. For example, at a droplet velocity of 3 m/s, predicted retention of Formulation 2 (Ecoteric T20) on a wheat leaf reduced from 100% with a droplet size of 100µm down to 12.9% with a droplet size of 700µm (Table 3). Increasing the velocity from 3m/s to 9 m/s for a 100µm drop of Formulation 2 on a wheat leaf reduced the retention from 100% down to 15%.

The main reason for this trend is that larger and faster droplets have greater energy on impact. For a given leaf surface, as the energy of the impacting droplet increases, the velocity of any resulting rebound or shatter droplet increases. The faster these rebound and shatter droplets move, the greater the chance that they move further from the point of impact and hence are not retained on the leaf of original impact, although they may be retained on other nearby leaves if they are present. These results indicate that the velocities and direction of drops after initial impact can influence the final retention on the leaf. Further work is required to refine and validate this effect.

5.2 Leaf characteristics

Predicted retention on cotton leaves was much higher than on chenopodium and wheat. At a velocity of 3 m/s, all droplet sizes and formulations tested on cotton adhered on impact, so retention was 100% (Table 4). This can be contrasted to retention of 400µm droplets of Formulation 1 (water) and Formulation 2 (Ecoteric T20), where all droplets bounced off a chenopodium leaf after initial impact, so retention was 0% (Table 4). The lowest predicted retention on cotton leaves was 43.2% for 700 µm droplets at a velocity of 9m/s (Table 2), whereas retention on chenopodium was often below 10% (Table 4). The average predicted total retention across all droplet size, velocity and formulations scenarios tested was 85, 30 and 18% for cotton, wheat and, chenopodium respectively.

This result is largely due to the easy to wet nature of cotton leaves, as reflected in lower static contact angles and high K_{crit} values (Table 1). There is also a tendency when droplets shatter or bounce for retention to be higher as leaf surface area increases (leaf areas for cotton, wheat and chenopodium were 2,848, 1,848 and 731mm² respectively). After initial impact any shatter or bounce droplets move away from the point of impact and hence the larger the surface area, the greater the proportion of shatter and bounce droplets likely to be intercepted.

5.3 Formulations

Retention of spray on leaf surfaces can be modified by changing the properties of the formulation applied. Reducing the surface tension of the liquid generally reduces the static contact angle of the formulation on the leaf surface, resulting in higher retention. For example, retention of 400 μm droplets on chenopodium at a velocity of 3 m/s reduced from 46.8% for Formulation 3 (Pulse) down to 0.0% for Formulation 1 (water) and at 9 m/s reduced from 16.4% down to 1.1% (Table 2).

This increase in retention, achieved by modifying formulation properties, was most notable on the hard to wet species of chenopodium and wheat. The repulsion of shatter droplets increases as the contact angle between droplet and leaf increases. Hence retention values are lower with Formulation 1 (water) than with Formulation 3 (0.1% Pulse) on all three leaf types since the greater the velocity the further the droplets are propelled away from the point of impact.

5.4 Leaf model detail

It was found that increasing the detail in the leaf model through using a finer mesh slightly increased the predicted retention on the chenopodium leaf (Table 5). Increasing the amount of detail however increases the run time of the model. This becomes more significant when extending the model to whole plant and full field applications. The same trends and comparative differences in retention were observed between the fine and coarse mesh and the difference in predicted retention was often less than 2%. Given the relatively small difference compared to the greater run time it is considered that the coarse mesh leaves would be suitable for future studies with full plants.

6 Conclusions

A model to predict spray retention on leaf surfaces based on scanned leaf images and measured formulation properties has been developed. The results show that incoming droplet properties (size and velocity), spray formulations, leaf surface characteristics and properties of any shatter or bounce droplets after impact, all influence the amount of spray retained on a leaf surface. Formulations with a lower surface tension and static contact angle on a leaf surface will result in higher retention. Retention was found to decrease with increasing droplet size and velocity for a given formulation and leaf type.

The droplet impaction models described in this paper are for a combination of horizontal leaves and droplets impacting perpendicular to the surface. Further work is required to allow droplets to impact the leaf at different angles. The shatter model needs to be improved in the area of the predicted number of shatter drops generated, velocity of these satellite drops and their trajectory.

Ultimately, the impaction model will be incorporated into virtual models of commercially relevant crop and weed plants that are currently being developed, followed by laboratory and field validation of the results. These simulations will then be used to quantify agrichemical spray retained by the foliage, and its relative distribution through the plant canopy for the sustainable management of pesticides in agricultural systems.

Acknowledgements

The authors acknowledge support from the Australian Research Council through the ARC Linkage Project LP100200476 and its industry partners, Syngenta, Dow AgroSciences, Croplands/NuFarm, Bill Gordon Enterprises and Plant Protection Chemistry NZ Ltd.

References

Arcange, R., de Silanes, M.C.L., Torrens, J.J. (eds.) 2004. Multidimensional minimising splines. Springer.

Attane, P., Girard, F., Morin, V., 2007. An energy balance approach of the dynamics of drop impact on a solid surface. Physics of Fluids 19, 1-17.

Bergeron, V., Martin, J.Y., Vovelle, L., 1999. Interaction of droplets with a surface: Impact and adhesion. Agro Food Industry Hi-Tech 10, 21-23.

Dorr, G., 2009. Minimising Environmental and Public Health Risk of Pesticide Application Through Understanding the Droplet-Canopy Interface. The University of Queensland, Ph.D. thesis.

Dorr, G., Hanan, J., Adkins, S., Hewitt, A.J., O'Donnell, C., Noller, B., 2008. Spray deposition on plant surfaces: a modelling approach. Functional Plant Biology 35, 988-996.

Forster, W.A., Kimberley, M.O., Steele, K.D., Haslett, M.R., Zabkiewicz, J.A., 2006. Spray Retention Models for Arable Crops. Journal of ASTM International, 3.

Forster, W.A., Kimberley, M.O., Zabkiewicz, J.A., 2005. A universal spray droplet adhesion model. Transactions of the ASABE 48, 1321-1330.

Forster, W.A., Mercer, G.N., Schou, W.C., 2010. Process-driven models for spray droplet shatter, adhesion or bounce. , in: Baur, P., Bonnet, M. (Eds.), 9th International Symposium on Adjuvants for Agrochemicals. ISAA Society, The Netherlands, pp. 277-285.

Kempthorne, D.K., Turner, I.W., Belward, J.A., 2012. Computational strategies for surface fitting using thin plate spline finite element methods in: McCue, S.W., Moroney, T., Mallet, D., Bunder, J. (Eds.), Proceedings of the 16th Biennial Computational Techniques and Applications Conference, pp. C56-C71.

Kempthorne, D.K., Turner, I.W., Belward, J.A., 2013. A Clough-Tocher Thin Plate Spline Smoother with Application to Virtual Leaf Construction. SIAM Journal on Scientific Computing In Review.

Loch, B., 2004. Surface fitting for modelling the development of plant leaves. The University of Queensland, Ph.D. thesis.

Mao, T., Kuhn, D.C.S., Tran, H., 1997. Spread and rebound of liquid droplets upon impact on flat surfaces. AIChE Journal 43, 2169-2179.

Marmanis, H., Thoroddsen, S.T., 1996. Scaling of the fingering pattern of an impacting drop. Physics of fluids 8, 1344-1346.

Mech, R., 2005. CPFG version 4.0 user's manual. http://algorithmicbotany.org/lstudio/CPFGman.pdf.

Mercer, G.N., Sweatman, W., Elvin, A., Harper, S., Fulford, G., Caunce, J.F., Pennifold, R., 2007. Process driven models for spray retention by plants, in: Wake, G.C. (ed.), Proceedings of the 2006 Mathematics in Industry Study Group. Massey University.

Mercer, G.N., Sweatman, W., Forster, W.A., 2010. A model for spray droplet adhesion, bounce or shatter at a crop leaf surface. Progress in Industrial Mathemattics at ECMI 2008. Mathematics in Industry 15, 945-951.

Moreira, A.L.N., Moita, A.S., Panao, M.R., 2010. Advances and challenges in explaining fuel spray impingement: How much of single droplet impact research is useful? Progress in Energy and Combustion Science 36, 554-580.

Mundo, C., Sommerfeld, M., Tropea, C., 1995. Droplet-wall collisions: Experimental studies on the deformation and breakup process. International Journal of Multiphase Flow 21, 151-173.

Mundo, C., Tropea, C., Sommerfeld, M., 1997. Numerical and experimental investigation of spray characteristics in the vicinity of a rigid wall. Experimental Thermal and Fluid Science 15, 228-237.

Oqielat, M.N., Turner, I.W., Belward, J.A., McCue, S.W., 2011. Modelling water droplet movement on a leaf surface. Mathematics and Computers in Simulation 81, 1553-1571.

Pathan, A.K., Kimberley, M.O., Forster, W.A., Haslett, M.R., Steele, K.D., 2009. Fractal characterisation of plant canopies and application in spray retention modelling for arable crops and weeds. Weed Research 49, 346-353.

Prusinkiewicz, P., 2004. Modelling plant growth development. Current Opinion in Plant Biology 7, 79-83.

Prusinkiewicz, P., Karwowski, R., Lane, B., 2007. The L+C plant-modelling language, in: Vos, J., Marcelis, L.F.M., de Visser, P.H.B., Struik, P.C., Evers, J.B. (eds.), Functional-structural plant modelling in crop production. Springer, pp. 27-42.

Schou, W.C., Forster, W.A., Mercer, G.N., G.N., T., Thistle, H.W., 2012. Building canopy retention into AGDISP: Preliminary models and results. Transactions of the ASABE 55, 2059-2066.

Sikalo, S., Tropea, C., Ganic, E.N., 2005. Impact of droplet onto inclined surfaces. Journal of Colloid and Interface Science 286, 661-669.

Teske, M.E., Bird, S.L., Esterly, D.M., Curbishley, T.B., Ray, S.L., Perry, S.G., 2002. AgDRIFT (R): A model for estimating near-field spray drift from aerial applications. Environmental Toxicology and Chemistry 21, 659-671.

Turner, I.W., Belward, J.A., Oqielat, M.N., 2010. Error Bounds for Least Squares Gradient Estimates. SIAM Journal on Scientific Computing 32, 2146-2166.

Yoon, S.S., DesJardin, P.E., 2006. Modelling spray impingement using linear stability theories for droplet shattering. International Journal for Numerical Methods in Fluids 50.

Yoon, S.S., DesJardin, P.E., Presser, C., Hewson, J.C., Avedisian, C.T., 2006. Numerical modelling and experimental measurements of water spray impact and transport over a cylinder. International Journal of Multiphase Flow 32, 132-157.

Zabkiewicz, J.A., 2007. Spray formulation efficacy—holistic and futuristic perspectives. Crop Protection 26, 312-319.

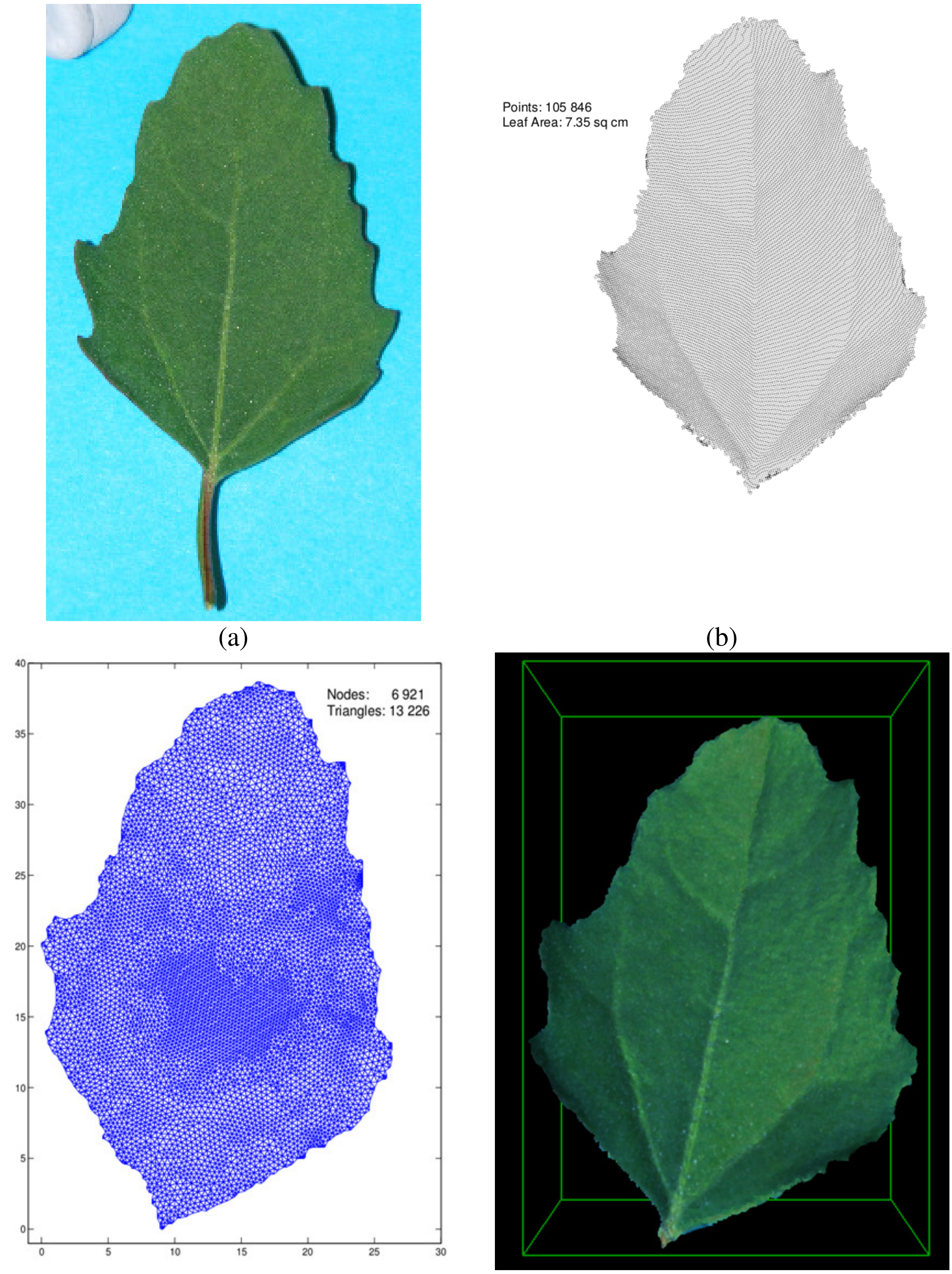

Figure 1 (a) Photograph of a chenopodium leaf with area 735 mm^2 (b) Point cloud of the scanned leaf (c) Generated mesh and (d). The resultant model leaf surface.

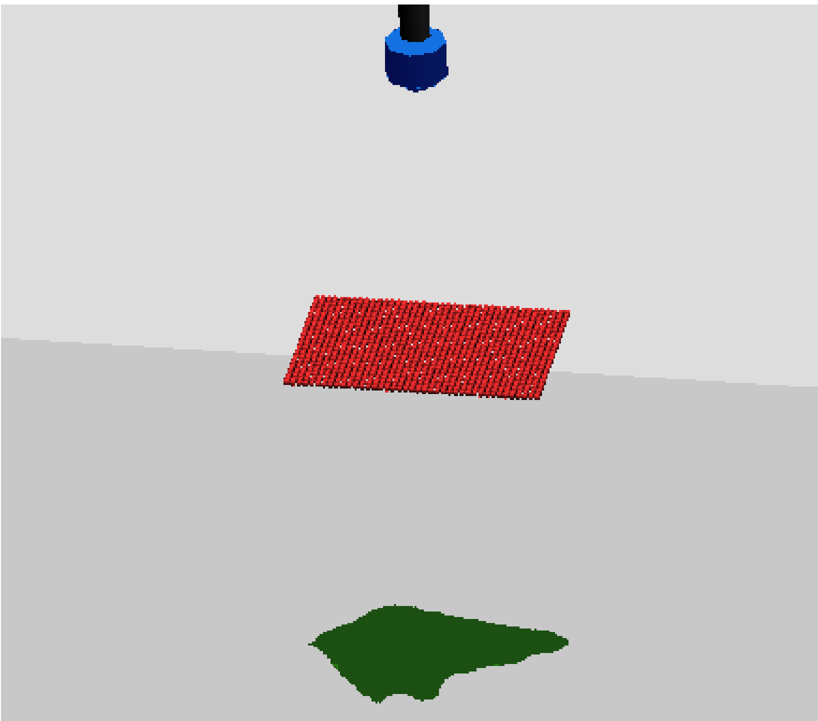

Figure 2. L-studio screen shot showing a grid of droplets falling onto a chenopodium leaf.

Video (for electronic version)

Video 1. L-studio animation showing 200um drops at 3m/s of Form 3 (0.1% Pulse) adhering on impact with a chenopodium leaf (Form3-200um-3mps.mov)

Video 2. L-studio animation showing 200um drops at 3m/s of Form 1 (water) bouncing on impact with a chenopodium leaf (Form1-200um-3mps.mov)

Video 3. L-studio animation showing 200um drops at 9m/s of Form 1 (water) shattering on impact with a chenopodium leaf (Form1-200um-9mps.mov)

Table1. Physical properties used in model

	Form 1			Form 2			Form 3		
Mixture	100% Water			0.1% Ecoteric® T20			0.1% Pulse®		
Plant	Ch	Wh	Co	Ch	Wh	Co	Ch	Wh	Co
Surface Tension (N/m)	0.073	0.073	0.073	0.048	0.048	0.048	0.023	0.023	0.023
Static Contact Angle (°)	179[a]	179 [a]	1[b]	131	129	1[b]	1[b]	1[b]	1[b]
K_{Crit}	52	65	150	52	65	150	52	65	150

Ch - chenopodium, Wh - wheat, Co - cotton

[a] There was complete repulsion of the droplet, so a value of 179 was used

[b] There was complete spreading, so a value of 1 was used.

Table 2. Predicted retention of spray on a single horizontal cotton leaf

Droplet Size (µm)	Predicted retention (% of the total volume of spray droplets impacting the leaf)											
	Velocity=1m/s			Velocity=3m/s			Velocity=6m/s			Velocity=9m/s		
	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3
100	100	100	100	100	100	100	100	100	100	100	100	100
200	100	100	100	100	100	100	100	100	100	100	100	78.6
300	100	100	100	100	100	100	100	100	100	100	67.3	70.2
400	100	100	100	100	100	100	100	100	68.6	56	58.2	61.4
500	100	100	100	100	100	100	100	100	63.8	49.9	51.4	53.7
600	100	100	100	100	100	100	100	57.7	60	45.5	46.8	48.8
700	100	100	100	100	100	100	99.3	54.8	55.8	43.2	44.5	45.7

Primary adhesion | Bounce + recapture | Shatter + recapture

Table 3. Predicted retention of spray on a single horizontal wheat leaf

Droplet Size (µm)	Predicted retention (% of the total volume of spray droplets impacting the leaf)											
	Velocity=1m/s			Velocity=3m/s			Velocity=6m/s			Velocity=9m/s		
	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3
100	100	100	100	27.7	100	100	15.6	17	100	9.6	15	58.4
200	100	100	100	14.4	15.6	100	3	42.8	52.9	21	45	50.6
300	100	100	100	12.0	13.3	100	14	24.2	48.5	13.6	26.5	47
400	100	100	100	6.0	12.2	54.8	11.2	15.4	47.6	11.4	13.9	45.4
500	28.3	100	100	2.8	11.8	53.4	10.8	12.9	47.5	10.9	11.5	44.2
600	16.1	100	100	2.4	13.6	53.1	10.8	11.3	45.9	10.1	11	44.2
700	13.5	38.8	100	2.2	12.9	53	7.3	11.5	45.8	5.3	10.4	43.8

Primary adhesion | Bounce + recapture | Shatter + recapture

Table 4. Predicted retention of spray on a single horizontal chenopodium leaf (coarse mesh)

Droplet Size (µm)	Predicted retention (% of the total volume of spray droplets impacting the leaf)											
	Velocity=1m/s			Velocity=3m/s			Velocity=6m/s			Velocity=9m/s		
	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3	Form 1	Form 2	Form 3
100	100	100	100	51.4	99.1	100	10.7	16.5	100	5.9	29.8	50.8
200	100	100	100	2.3	6.7	100	13.3	16.4	39.1	5.7	16.1	33.0
300	100	100	100	0.0	0.7	51.3	2.3	11.1	26.5	1.5	5.2	20.2
400	100	100	100	0.0	0.0	46.8	1.1	2.7	21.0	1.1	2.4	16.4
500	51.4	100	100	0.0	5.2	42.8	1.3	1.8	18.6	1.0	1.3	15.2
600	36.9	83.9	100	1.6	2.3	41.4	1.2	1.5	17.6	1.0	1.4	14.7
700	26.5	54.6	100	1.2	1.8	39.8	0.9	1.2	16.6	0.6	1.2	14.5

Primary adhesion | Bounce + recapture | Shatter + recapture

Table 5. Comparison of fine and coarse chenopodium leaf mesh surface on retention at 3m/s velocity.

Droplet Size (µm)	**Retention (% of spray droplets impacting the leaf)**					
	Form 1		Form 2		Form 3	
	coarse	fine	coarse	fine	coarse	fine
100	51.4	51.9	99.1	100	100	100
200	2.3	7.2	6.7	10.6	100	100
300	0.0	3.7	0.7	6.3	51.3	53.1
400	0.0	1.1	0.0	4.3	46.8	47.1
500	0.0	1.6	5.2	5.8	42.8	44.3
600	1.6	1.9	2.3	3.1	41.4	42.3
700	1.2	1.9	1.8	2.7	39.8	40.6

Primary adhesion   Bounce + recapture   Shatter + recapture