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Spray retention on whole plants: modelling, simulations and experiments

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

[a] The University of Queensland, Queensland Alliance for Agriculture and Food Innovation, Brisbane, Australia
[b] Plant Protection Chemistry NZ Ltd, Rotorua, New Zealand
[c] School of Mathematical Sciences, Queensland University of Technology, Brisbane, Australia
[d] High Performance Computing and Research Support, Queensland University of Technology, Brisbane, Australia
[e] SciCon Scientific Consultants Ltd, Rotorua, New Zealand

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ABSTRACT

Retention of sprays on plants is a critical component influencing the effectiveness of agrichemical applications. Previous simulations of **s**pray retention by plants gave poor agreement for hard-to-wet species when compared with actual measured retention. A new model is developed here that accounts for: species wettability, impaction angle, droplet bounce, partial retention on shatter, a variable time to shatter, and the number of daughter droplets produced. The aim of this study was to compare predictions from the new model with data obtained by spraying five mixtures via five nozzles onto easy-to-wet cotton (*Gossypium hirsutum* L.), and hard-to-wet wheat (*Triticum aestivum* L.) and fat hen (*Chenopodium album* L.). The new model correctly predicts retention to be highest on cotton and lowest on wheat. The trend in both measured data and the model predictions is for retention to decrease with increasing droplet size, on all three plant species. Formulation is correctly predicted to have little influence on retention by easy-to-wet cotton plants and to enhance retention by the harder-to-wet wheat and fat hen plants. The parameters that describe partial retention on shatter and variable time to shatter have a substantial influence on retention, as they affect primary or secondary droplet capture. A better understanding of the kinetic energy effects and the interactions between the formulation and the leaf surface are needed to refine their input values.

1. Introduction

Efficient spray application is essential in today's environmentally sensitive world. Much effort has gone into developing minimum spray drift application and formulation technologies so that spray deposition within the target spray area is generally high, with only minimal amounts of off-target spray drift. However, within the target area, the efficiency of spray retention by the plants may be quite varied. High retention on plants is important, as the deposition of the non-retained proportion onto the soil is often a total waste of product and a potential environmental contaminant.

Pesticide application research is normally undertaken using field experiments that are conducted under prevailing meteorological conditions. However, it is often difficult, time consuming and expensive to conduct numerous field experiments because of the variability and complexity involved.

Alternative approaches, including the use of wind tunnels or spray chambers, are therefore often employed to allow experiments to be performed under repeatable and controllable conditions. This makes it possible to perform multiple experiments over short time periods and similar air flow conditions, which is not possible in the field. These alternative experimental approaches can provide large amounts of reliable data and are often the most rapid, economical and accurate means for conducting fundamental research (Barlow et al., 1999).

* Corresponding author. School of Mathematical Sciences, QUT, Brisbane QLD 4001, Australia.
E-mail address: scott.mccue@qut.edu.au (S.W. McCue).

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Theoretical models and computer simulations have also been used to estimate the likely deposition of pesticides onto plants or soil surfaces (Butler Ellis and Miller, 2010; Teske et al., 2002) and to improve understanding of the pesticide spray application and behaviour processes. Virtual plant architectural models can position various plant components in three-dimensional space (Prusinkiewicz, 2004b) and, when combined with particle trajectory models, make it possible to effectively study the retention of impinging spray droplets onto such vegetative elements (Dorr et al., 2008). The use of computer simulations enables strong and fundamental links to be made between the pesticide application process, the influence of plant architecture and leaf surface characteristics, and spray formulation properties on the pesticide retention and canopy distribution pattern. This theoretical approach can substantially improve our understanding of the complex relationships causing the retention of pesticide droplets on vegetative surfaces (e.g. crop canopy, weeds, downwind buffer vegetation) and has the potential to estimate the distribution of pesticides within a plant canopy at very low costs in time and materials.

Compared to undertaking a set of experiments in the field, running a virtual experiment through mathematical models and computer simulations is fast and reproducible. As a general rule, such mathematical models should include as much physics and chemistry as is necessary to describe the important processes involved, but should not be overly complicated or contain too many input parameter values. In the present context, the models should also be simple enough to facilitate simulations with tens of thousands of droplets impacting on leaf surfaces using standard desktop computing resources. Ultimately, models need to be suitably tested by verifying the correctness of an algorithm or code and validating the results by comparing model outputs with actual physical measurements (Haefner, 2005).

Previous research has resulted in models for initial adhesion and spray retention (Dorr et al., 2014; Forster et al., 2005, 2006) by individual leaves and plants. These models utilise parameters that describe solution properties, fluid properties of the spray droplets, and leaf surface characteristics. A combined spray and plant architecture model used (Dorr et al., 2008) to investigate retention by plants showed good agreement between the model and experimental results for *Gossypium hirsutum* L. (cotton; an easy-to-wet plant), but retention measured on *Sonchus oleraceus* L. (sow thistle; hard-to-wet) plants was lower than predicted by the model. The suggested reasons for the lower than predicted deposit on sow thistle were that droplet bounce was not taken into account and shatter equations were based on simple empirical relationships that are only valid for easy-to-wet surfaces. A further analysis of the model (Dorr, 2010) concluded that formulation effects such as surface tension did not have a significant effect on the modelled spray retention. While this conclusion may be valid for easy-to-wet plants on which the model assumptions were based, it is not true for hard-to-wet plants (Bruns and Nalewaja, 1998; de Ruiter et al., 1990; Hall et al., 1997).

In this paper, a multi-component predictive spray retention model is described and its predictions are compared with experimental results obtained from spraying: three plant species, ranging from easy-to-wet (cotton) to hard-to-wet (*Triticum aestivum* L. and *Chenopodium album* L.; wheat and fat hen respectively); with five spray mixtures (static surface tensions ranging from 22 to 72 mNm^{-1} and dynamic surface tension at 50 ms ranging from 55 to 72 mNm^{-1}); applied through five different commercially available agrichemical spray nozzles (which produced droplets ranging in $D_{v0.5}$ from 202 μm to 833 μm with water).

2. Materials and methods

2.1. Predictive spray retention model

2.1.1. Spray model

The combined spray and plant architectural model utilised in this study is based on the model described by Dorr et al. (2008) and developed in L-studio (Prusinkiewicz, 2004a; Prusinkiewicz et al., 2007), a Windows-based software environment for creating plant-based simulation models. A particle trajectory model, based on the combined ballistic and random walk approach proposed by Mokeba et al. (1997) and Cox et al. (2000), is implemented to model the movement of droplets through the air from the nozzle to the target plant. In this model, time is divided into a large number of small, discrete steps, during which the velocity of the particle is kept constant. The movement of individual droplets through the atmosphere is tracked through successive time steps. A meaningful estimate of dispersal statistics can be obtained by following a large number of trajectories (Butler Ellis and Miller, 2010; Hashem and Parkin, 1991).

2.1.2. Plant model

The plant models for this study were developed for cotton, fat hen and wheat using the L-system formalism (Prusinkiewicz, 2004b; Prusinkiewicz et al., 2000) and incorporated into the main model as sub L-systems (Mech, 2005). The structure of the cotton model is based on existing functional–structural models of cotton (Room and Hanan, 1995), but the cotton leaves in that model are replaced with actual scanned and reconstructed cotton leaves (Dorr et al., 2014; Kempthorne et al., 2014a, 2014b). The algorithm for the plant model was allowed to run for nine iterations, resulting in a plant with 13 leaves. Fat hen and wheat models are based on physical measurements of plants grown in pots under prevailing weather conditions. Individual leaves in the model are obtained from scanned and reconstructed leaves (Kempthorne et al., 2015).

2.1.3. Impaction models

Droplet retention models for bounce and shatter (Dorr et al., 2014), expanded to include oblique impact angles (Dorr et al., 2015), have been incorporated into the current model. These consider droplet impaction events individually, and employ traditional energy balance principles that enforce energy and mass conservation at key stages of the impaction process. Such energy balance models have been widely used as a simple and computationally tractable approach to describe droplet impact (Attane et al., 2007; Bechtel et al., 1981; Kim and Chun, 2001; Mao et al., 1997; Yoon and DesJardin, 2006).

The impaction models employed in the current work are purely algebraic (i.e., they do not require the solution of differential equations, as has been the approach in many other energy models (Attane et al., 2007; Bechtel et al., 1981; Kim and Chun, 2001)). This is a deliberate choice, as the full spray retention model has many components and can become very computationally intensive and beyond standard desktop capabilities as the number of droplets becomes large. Therefore, we have taken the liberty to use very simple and idealised models for bounce and shatter that can be generalised to any new spray scenario. The intention is to work towards impaction models that are not only efficient, but are formulated in a process-oriented way which minimises the need for empirical fitting. Alternatively, several recent studies have used experimental fitting to produce a probabilistic method for predicting adhesion, bounce, and shatter (Massinon et al., 2014; Massinon and Lebeau, 2012; Zwertvaegher et al., 2014). These models were then utilised within a 3D virtual spray model similar to ours to study the retention of water and a low surface tension