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Chapter 13A

Modeling of Pesticide Application, Deposition and Drift

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Abstract: Applied modeling techniques describing simulation of ground spraying and aerial spraying of pesticides are presented. The state of the art in aerial spraying is somewhat further advanced due to early concerns about off-target drift of aerially applied pesticide sprays. Recent regulatory concern has focused on drift from ground sprayers and has initiated a body of model development work that is currently very active. Modeling of pesticide application generally divides the model domain into regions 1) where the machine and wake effects dominate and 2) where material movement is dominated by ambient environmental conditions. Though well over 30 environmental and mechanical variables have some influence on droplet (or particle) landing position, the primary dependence is with particle size. The existing models have focused on liquid spraying and are generally not atomization models but require a droplet size distribution to be input. The droplet distribution is binned by size and various mathematical schemes are used to transport the released droplets to the position of deposit. Droplet evaporation can be a critical variable in the case of materials with high volatility, so droplet evaporation is described. Models typically will incorporate a scheme to describe the interaction with the target surface (vegetative or otherwise). These schemes must include a description of collection efficiency or 'likelihood' that an approaching droplet will deposit. Ground sprayer modeling must also consider droplet plume interaction with horizontal obstacles in an aggregate sense.

Key Words: pesticide deposition, pesticide application modeling, Lagrangian droplet transport, ground spraying, aerial spraying, pesticide spraying, pesticide drift.

1 Introduction

Modeling of pesticide application is undertaken for many of the reasons that most physical modeling is performed. That is, to create a simulation that can be manipulated with respect to the modeled variables at much lower cost than replicating field measurements. Mechanistic models of the type emphasized here can also be used to gain insight to the basic physical phenomena being modeled, test sensitivity to the relevant mechanistic and physical variables, and point out data gaps in our understanding of the underlying relationships.

The models that have developed and evolved (in the sense of having been written and then altered in response to new information and technologies) in the area of pesticide application modeling are mechanistic models but generally do not attempt to be full physics models. For example, though the spray drop size distribution is most often the primary determinant of the landing position of the spray mass, the models described here do not typically tackle the difficult problem of primary atomization. Instead, measured initial droplet spectra are input based on user knowledge of nozzle type, nozzle angle relative to the vehicle movement (the slipstream) etc. The models described below typically use Lagrangian droplet transport schemes but may also incorporate Gaussian elements as well as simple volume dilution approximations (box models).

In the context of this chapter, it is worth noting that pesticide application models can often account for the landing position of a large part of the released mass with an accuracy that might leave some atmospheric dispersion modelers incredulous. It must be remembered that if a slow moving tractor (say 15 km/hr forward speed) is releasing 600µm droplets from a boom .6 m above the ground surface, gravity will often put a large majority of the mass in the tractor 'swath' in a relatively predictable manner. Even in this scenario, the various shear forces associated with atomization, wake and atmospheric forces will conspire to produce some fine droplets and move them away from the spray target. It is the challenge of the modern pesticide application modeler to anticipate the fate of smaller and smaller amounts of spray material at greater distances as scrutiny of pesticide application, and concerns about pesticide residue continue to increase.

The development of pesticide application modeling has been driven by regulatory applications. Regulators need relatively simple, consistent tools to determine exposure to pesticides in scenarios ranging from human health to ecotoxicity. In the United States, pesticide use is regulated through label language printed on labels affixed to the pesticide container. Approval of label content and the decision to allow a pesticide on the market for use rests with US EPA and is based on a comprehensive registration process that includes extensive risk assessment. Pesticide application and fate models are used in a formal process as part of pesticide registration. In other countries, pesticide application models are used to set buffers or setbacks that cannot be sprayed into directly. These buffers are often established using pesticide application modeling. In the United States, pesticide application models are increasingly used by government agencies enforcing the endangered species act. Using ecotoxicity data for specific endangered species and specific chemicals, 'no spray' buffer zones are established around endangered creatures to protect them from deleterious effects due to pesticides. Other regulatory applications of modeling include regulating the types of pesticides that can be used in a given scenario, and the number of times application can occur in a given time period, as well as other application parameters.

This chapter deals with primary drift, which is drift from the sprayer to droplet landing position. A vapor phase exists as liquid droplets evaporate, and this primary vapor drift is not discussed in detail here. Reentrainment, volatilization from surfaces after deposition, etc., known as secondary drift, is not discussed. Formulation chemistry is a field in itself and the chemistry of the spray material is a controlling factor in liquid atomization. Chemicals introduced to improve application efficacy and reduce drift are known as adjuvants and these present a myriad of options to the applicator. Much formulation chemistry is proprietary. To keep modeling manageable, the models generally only need droplet size distribution, volatility and specific gravity specified. If it is believed that the chemistry affecting the position of spray deposition is not adequately described using these properties, wind tunnel droplet sizing must be undertaken with the actual spray mixture used to determine the droplet size spectra. Since the droplet size spectra is the primary determinant of landing position, increasing droplet size is often the goal in drift reduction.

It is difficult to generalize the approaches described here to all spraying scenarios. Two that are recognized by the modeling community as distinct from aerial and ground as described below are orchard air-blast, and public health spraying. Orchard air blast utilizes fine droplets propelled into orchard canopies (often upward) using a strong air stream as the carrier. Though modeling approaches have been proposed for this scenario (see Walklate (1987) and Cross et al. (2001a, 2001b, 2003) for an example of a modeling approach and basic variable interactions) these have not yet been developed into user models and are not discussed here. Public health aerial applications (mosquito control) release ultra-fine droplets either by air or ground with the objective being spray moving through a target volume of air. Moreover, aerial applications are released from high altitudes (30-75m). The aerial modeling techniques described in this chapter have been extensively used by the mosquito adulticiding community, but should be done so with caution as this use requires calculations outside the spatial domain of this model.

Finally, the scope of this short chapter precludes it being a primer on pesticide application. Actual application scenarios range from 1500 μm droplets used for herbicide application from low boom ground sprayers to aerosol droplets being released at a 75m height in an attempt to cause a droplet to encounter a flying mosquito in the air (known as adulticiding). The reader is referred to Matthews

(1992), Picot and Kristmanson (1997) and Kilroy et al., (2003) among many other references for overviews of pesticide application methods and equipment.

2 Sprayer Types

Conventional sprayers for making pesticide applications to ground (field) crops generally consist of a boom that is typically 6.0 to 24.0 m wide (exceptionally up to 42.0 m wide) and constructed of standard steel or aluminum sections in such a way that nozzles can be supported at a constant height above the crop canopy along the length of the boom. Smaller machines are vehicle mounted with tank sizes up to 2000 L also mounted around the vehicle. Larger machines are commonly self-propelled typically with tank sizes from 2000 to 5000 L but exceptionally with tanks larger than this. In Europe, Australia and New Zealand most boom sprayers for use in field crops are fitted with 110^{o} flat fan hydraulic pressure nozzles whereas in the Americas the use of 80^{o} and some hollow cone nozzles is more common. The fan nozzle has the advantage of giving a uniform volume distribution pattern over a wide range of heights and, for 110^{o} nozzles spaced at 0.5 m on the boom (a common configuration), the minimum boom height is between 350 and 500 mm above the crop depending on the design of the nozzle. Machines are typically operated at speeds from 5.0 to 25.0 km/h, the lower speeds being used in some European countries and higher speeds in Australia, Canada and the USA. The machines are used to apply volumes in the range 50 to 400 L/ha with the lower volumes giving advantages in terms of work rate due to the reduced time required to fill the machine.

Aerial spraying can be performed with either fixed or rotary wing aircraft. Fixed wing are often preferred in open terrain where higher speed flying reduces application costs, while helicopters are preferred where maneuverability or slow airspeeds are required. Such scenarios might include mountain spraying or spraying small areas. Though larger airplanes, such as C-130s are used in applications such as mosquito control, typical examples of the larger fixed wing aircraft commonly used in crop and forestry applications are the Air Tractor AT 602 and 802. The 802 has a useful load of over 4000 kg. In some applications, the actual ratio of active ingredient to carrier may be 1% or less but due to the extra cost of carrying additional weight and refilling, more concentrated solutions are used in aerial application when possible. Aerial herbiciding of low canopies may be done with coarse sprays (>350 µm volume median diameter (VMD)) while spraying deep, three-dimensional canopies such as forests with insecticides, might require a very fine spray (100 µm VMD). While most aerial spraying is done with hydraulic nozzles, much insecticide spraying is done with rotary atomizers utilizing a spinning cage to create fine sprays. An AT-802 fixed wing aircraft might work at airspeed of 230 km hr^{-1} but most aircraft will work at somewhat lower speeds. The Bell 47G helicopter might cruise near 140 km hr^{-1} but can work at speeds down to hover as is desirable in certain specialty applications.

Two linked videos show a Bell47G3-B2A helicopter spraying a dye to evaluate the role a riparian barrier plays in preventing spray drift to a stream running within the barrier strip. These trials were conducted using electronically driven rotary atomizers producing a droplet Volume Median Diameter (VMD or $D_{V.0.5}$) of 126 μm (test details in Thistle et al, 2009). These videos illustrate some of the influences on spray movement discussed in this chapter. The first video (Trial04.wmv) shows the helicopter flying along the barrier edge releasing spray at a height of 15.2 m, with mean wind velocity toward the barrier at 2.8 ms^{-1}, temperature at 19.5 °C and relative humidity of 41%. The Pasquill stability index is D in this trial. Note the spray capture in the vortices and the downward motion of the vortices while the ambient air motion moves the vortices laterally and degrades vortex coherence. Also, note that at low humidities, the droplet VMD is rapidly decreasing after release from the aircraft due to evaporation. In the second video (Trial13.wmv), release height is 11.3m, the mean wind velocity lacks consistent direction and is at .7 ms^{-1}, temperature is .8°C and relative humidity is 88%. Importantly, the Pasquill stability index is F in this trial. The video clearly shows that in this low wind speed, low mixing environment, the vortices descend but linger and a haze of fine droplets remaining aloft can be seen (videos filmed by James Kautz, USDA Forest Service).

3 Ground Application

3.1 Near Field Effects

Prediction of droplet trajectories and spray movement associated with a boom sprayer is dominated by the proximity of the boom and nozzles to the ground. The boom is generally of a relatively aerodynamically porous characteristic but the blockage to the airflow in the region below the boom by the presence of the sprays is considerable. Studies examining the relative magnitude of aerodynamic effects associated with both the boom structure and sprays (Murphy et al. 2000) have shown that changes in boom structure profile had a much smaller effect on the risk of drift than changes to spray nozzle characteristics.

The air entrained within the spray structure is also important in determining droplet trajectories close to the nozzle, particularly when considering the interaction with a cross-flow of air. A combination of the natural wind and the forward motion of the sprayer generate this cross-flow. Initial approaches to the modeling of the dispersion of sprays from ground based boom sprayers ignored the conditions close to the nozzle and assumed that the behavior of droplets detrained from the spray structure would be dispersed by atmospheric turbulence from some arbitrary release condition. This dispersion was then predicted using random walk approaches (Thompson and Ley 1983) or Gaussian plume models (e.g. Schaefer and Allsop 1983). The random walk approach used by Thompson and Ley further developed by assuming that droplets leaving a hydraulic pressure nozzle initially behaved ballistically within the entrained air flow created by the spray (Miller and Hadfield 1989). Entrained air flow conditions were calculated based on relationships initially proposed by (Briffa and Dombrowski 1966) in which the air velocity along the axis of the fan jet was given by:

$$U_c = U_s \left[\frac{l_c}{h} \right]^{\delta^2 / 2k} \tag{3.1}$$

where U_s is the liquid sheet velocity immediately below the nozzle, l_c is the coherent length of the sheet, h is the distance from the nozzle, δ is a constant which for sprays into air takes a value of 0.4 and k is a dimensionless parameter that is a function of the thickness of the spray structure at right angles to the main spray fan and at a defined distance below the nozzle. Studies reported by Miller and Hadfield measured spray structures from photographs to determine initial values for the $\delta^2/2k$ parameter and then validated the initial predictions by measuring droplet velocities within the spray produced by typical agricultural nozzle conditions. Entrained air velocities within the spray were measured by monitoring droplets in the 40-80 μm size range. A value for $\delta^2/2k$ of 0.95 was shown to give a reasonable prediction of entrained air velocities within the spray and was assumed to be constant across the spray structure. The geometry of the air jet was then modified in studies reported by Hobson et al. (1993) to match that of the spray, although the basic model and predictions of entrained air velocity used methods similar to those of Miller and Hadfield.

The approach to the modeling of spray behavior and drift from boom sprayers reported by Miller and Hadfield was also further developed by Holterman et al. (1997). In this case the definitions of entrained air velocities built on the approaches initially identified by Smith and Miller (1994) and were assumed to vary depending on the position within the spray structure such that entrained air velocities were predicted from:

$$U_e\,(p,q,h) \quad = \quad U_{e,ax} \cdot \frac{1}{4} \quad (\cos\left(\frac{\pi p}{f_h\, p_o}\right)+1) \;\; (\cos\left(\frac{\pi q}{f_h\, q_o}\right)+1) \tag{3.2}$$

where p and q represent the two orthogonal distances from the axis parallel and at right angles to the spray fan, p_o and q_o represent the outer limits of the spray fan in the two directions, are proportional to h and dependent on the spray fan angle. f_h is an extension factor for entrained air outside of the spray structure and has taken values of between 1.2 and 1.8 based on empirical assessments of the spray geometry. The entrained air velocity down the axis of the spray jet, $U_{e,ax}$ was calculated using the same relationship as given in Equation 3.1 with the constant $\delta^2 / 2k$ set as a constant (k_e) with a value of 0.7.

Work reported by Teske et al., (2009) also used the details of the physical structure and entrained air conditions associated with the liquid spray jet to improve upon the predictions of spray dispersion and drift from a ground sprayer using a Gaussian plume model. This work found that a value for the $\delta^2/2k$ parameter in Equation (3.1) of 0.57 gave reasonable predictions for sprays from conventional flat fan nozzles but for air-induction nozzles the value needed to be increased to 2.04 and the agreement between measured and predicted drift deposition was less good than that for the conventional nozzle design. The authors suggested that further laboratory work is needed in order to give model input data for predicting the drift from this nozzle design.

Droplet and entrained air velocities within a spray are major factors influencing behavior both in terms of drift and deposition on target surfaces. The entrained air jet within a spray differs from a turbulent air jet in that the scale of turbulence is much lower in the spray driven air jet (Ghosh et al 1991; Ghosh and Hunt 1994) and the initial rate at which the air velocity decays with increasing distance is a function of $z^{-1/2}$ rather than z^{-1} that is more typical of air jet structures. The velocities of air and droplets in a spray can be expressed as (Miller et al 1996):

$$V_r^2 = V_{r0}^2 . \frac{r_0^2}{r^2} - \frac{K}{r^2}(V_l - V_{l0}) \text{ where } K = q_l(\Theta)\frac{\rho_l}{\rho_a} \tag{3.3}$$

for the entrained air, and

$$V_l = V_{l0}.e^{-\lambda(r-r_0)} \text{ where } \lambda = \frac{3C_D.\rho_a}{8a.\rho_l} \tag{3.4}$$

for the droplets, and where V_r is the radial component of air velocity from the nozzle, r is the distance from the nozzle, V_l the velocity of droplets, ρ_a and ρ_l are the density of the air and liquid respectively, Θ is half the spray fan angle, C_D is the drag coefficient and a is the radius of the droplet. The subscript 0 relates to the position at the end of the liquid sheet where the droplets are formed. The relationship in Equation 3.3 has a flow rate term (q_l), which is to be expected given that the air jet is driven by the exchange of momentum between the air and the liquid.

The structure of a spray fan below a fixed boom is such that the interaction with a cross-flow that may detrain small droplets that then drift is likely to be directional. Studies reported by Smith and Miller (1994) showed that the quantity of liquid detrained from a spray in wind tunnel conditions was more than eight times greater when the cross-flow was at right angles to the main spray direction compared to when the cross-flow was aligned with the fan. These results were compared with model predictions that included a geometrical description of both the spray and entrained air structures using relationships similar to those included by Holterman et al. (1997) and detailed in Equation (3.2).

The effective component of the cross-wind that can be associated with the forward motion of the sprayer acts at approximately right angles to the main axis of the spray. A fundamental analysis of such a cross-flow interaction by Ghosh and Hunt, (1998) identified up to four areas below a nozzle where the behavior of the flow regime was dependent on the ratios of droplet and entrained air velocities to that of the cross-flow as follows:

(i) a region immediately below the nozzle where the cross-flow is relatively weak in comparison with droplet and entrained air velocities and where the spray entrains the cross-flow and acts like a line sink for airborne material;

(ii) an intermediate region where the line sink effect weakens and the cross-flow starts to penetrate the spray structure with some detrainment of small spray droplets;

(iii) a zone where the cross-flow fully penetrates the spray structure and where substantial detrainment of the small droplet component in the spray occurs but where larger droplets still have a substantial component of their initial release velocity;

(iv) a final zone where all of the spray has slowed to relatively low velocities and where the action of the cross-flow results in the spray fan being deflected in the direction of the cross-flow.

Regions (i), (ii), and (iii) are those most relevant to the operation of boom sprayers in most conditions. These flow conditions were studied experimentally by Phillips et al. (2000) using both flow visualization techniques and measurements of the droplet size and airborne flux profiles downwind of single and multiple nozzle arrangements using a phase Doppler analyzer in wind tunnel conditions. The work of both Ghosh and Hunt and Phillips et al. show that the interaction of a spray jet with a cross-flow would result in a pair of axial vortices that then move with the cross-flow. It is likely that the presence of these vortex structures will have important implications for the dispersal of detrained small droplets in field conditions and for the characterization of spray nozzles in wind tunnel test conditions. The presence of vortices in the interacting spray jet and cross-flows have also been identified by a number of research teams examining the behavior of sprays with agricultural boom sprayers (e.g. Young 1991, Miller and Smith 1997), but to date little work has been conducted to define the effect that such structures may have on the downwind dispersion of sprays.

3.2 Obstacles to Droplets Moving Laterally

Vegetative boundaries at the edges of a field can provide an effective filter of airborne spray from boom sprayers with reductions in airborne flux of up to 90% (Hewitt 2001, Ucar and Hall 2001, Miller et al 2000, Miller and Lane 1999). The effectiveness of such structures in capturing airborne spray is likely to be a function of many parameters particularly the aerodynamic porosity of the structure. Dense structures will obstruct the flow and scouring of airborne spray will be limited to the front face of the boundary. Greater porosities will enable flow through the structure and the filtering of the airborne spray. Studies of such systems have been mainly experimental (De Schampheleire et al. 2008a and 2008b, Lazzaro et al. 2007) with some analytical and computational fluid dynamics approaches to support such measurements.

The capture efficiency of a vegetative boundary Δ_b has been defined by (Raupach et al 2001, Connell et al 2010):

$$\Delta_b = \frac{U_b}{U_h}(1-\tau^{ME}) \tag{3.5}$$

where U_b is the bleed velocity, U_h is the open field wind velocity, τ is the optical porosity, M the meander factor for air flowing through the wind break and E is the capture efficiency that is a function of Stokes Number and is related to leaf dimensions and droplet sizes as:

$$E = [\frac{S_t}{(S_t + 0.8)}]^2 \tag{3.6}$$

The Stokes Number S_t is given by

$$S_t = \frac{\tau U_0}{d_c} \tag{3.6a}$$

where U_0 is the droplet velocity, d_c is the characteristic dimension of a leaf and τ is the relaxation time that is given by $\tau = \rho d^2/18\mu$, where d is the droplet diameter, ρ is the density of the droplet and μ the viscosity of the air. Airborne spray profiles downwind of a boom sprayer do not have a uniform flux distribution with height and therefore Equation 3.5 can be modified (Connell et al 2010) to:

$$\Delta_b = A.k_1^{0.5} \cdot \frac{U_b}{U_h}(1-\tau^{ME}) \tag{3.7}$$

where A and k_1 are factors that account for the wind and airborne flux profiles. Results from predictions based on Equation 3.7 have been shown to approximately agree with field measurements (Connell et al 2010).

4 Aerial Application

Over the last twenty-five years a significant modeling and data collection effort has been undertaken by the USDA Forest Service and its cooperators to develop accurate, validated models that predict the behavior of pesticides applied by aerial application above forests (Teske et al. 1998b). The model most focused upon is the Lagrangian trajectory model AGDISP (Bilanin et al. 1989). An extensive field study (Hewitt et al. 2002) and model validation effort (Bird et al. 2002) confirmed the predictive capability of the Lagrangian computational engine that drives the model (Teske et al. 2003), to approximately 800 m downwind (Teske and Thistle 2003), and opened the door for improved solution handoff to Gaussian models (Teske and Thistle 2004a) and mesoscale atmospheric transport models (Allwine et al. 2002 and Thistle et al., 2008).

AGDISP is based on a Lagrangian approach to the solution of the spray material equations of motion, and includes simplified models for the effects of the aircraft wake and aircraft-generated and ambient turbulence. Reed (1953) first developed the equations of motion for spray material released from nozzles on an aircraft, exploring the role of the wingtip vortices. Vortex swirling behavior can be quantified by a simple model that, when combined with the local wind speed and with gravity, effectively predicts the motion of spray material released into it. The original AGDISP model included the innovative step of developing ensemble-averaged turbulence equations to predict the growth of the spray cloud during the calculations, eliminating the need for a random component in the solution procedure.

Figure 1. A Bell 47G3-B2A spraying a yellow fluorescent dye in water at a rate of 46.8 L ha^{-1} with a fine (VMD of 126 μm) droplet size distribution. Note the definite vortices generated at the rotor tips as delineated by the dyed spray (Thistle et al. (2009), photograph by Jim Kautz, USDA Forest Service).

In this same time period other researchers independently developed their own spray drift models, or contributed essential pieces to the modeling process. These authors include Williamson and Threadgill (1974), Bache and Sayer (1975), Trayford and Welch (1977), Frost and Huang (1981), Atias and Weihs (1984), Bragg (1986), Gaidos et al. (1990), Himel et al. (1990), Saputro and Smith (1990), and Wallace et al. (1995).

4.1 Solution Approach

Released spray material can be modeled as a discrete set of droplets, collected into categories, and called a drop size distribution. Each drop size category is defined by its volume average diameter and volume fraction, and is examined sequentially by the model. A Lagrangian approach is used to develop the equations of motion for discrete droplets released from the aircraft, with the resulting set of ordinary differential equations solved exactly from time step to time step. Droplet flight path, as a function of time after release, is computed as the mean droplet locations X_i for all droplets included in the simulation. The positive X direction is taken as the direction the aircraft is flying from; the Y direction is off the right wing as viewed from the pilot's seat; and the Z direction is vertical upward. The interaction of the released material with the turbulence in the environment creates turbulent correlation functions for droplet position and velocity $\langle x_i v_i \rangle$, velocity variance $\langle v_i v_i \rangle$, and position variance $\langle x_i x_i \rangle$, where x_i is the fluctuating droplet position, v_i is the fluctuating droplet velocity, and $\langle\ \rangle$ denotes ensemble average. The square root of $\langle x_i x_i \rangle$ gives the standard deviation σ of the droplet motion about the mean described by X_i.

The novel feature of the AGDISP methodology is that the dispersion of a group of similarly sized droplets (contained within each drop size category), resulting from turbulent fluid fluctuations in the atmosphere, is quantitatively computed within the wake of the aircraft as the group of droplets descends toward the surface. The Lagrangian equations governing the behavior of a droplet in motion may be ensemble averaged and written

$$\frac{d^2 X_i}{dt^2} = [U_i - V_i]\left[\frac{1}{\tau_p}\right] + g_i \tag{4.1}$$

$$\frac{dX_i}{dt} = V_i \tag{4.2}$$

where t is time, U_i is the mean local velocity, V_i is the mean droplet velocity, and g_i is gravity (0,0,-g). The drag force on the droplet is represented by the droplet relaxation time

$$\tau_p = \frac{4}{3}\frac{D\rho}{C_D \rho_a |U_i - V_i|} \tag{4.3}$$

where D is the droplet diameter, ρ is the droplet density, C_D is the droplet drag coefficient, and ρ_a is the density of air. The term representing the effect of evaporation on droplet acceleration has been removed from Equation (4.1) because its effect is small (droplet evaporation is described in detail in Section 4.2), and its presence significantly complicates the problem (and makes the later analytical solution impossible). C_D is evaluated empirically for spherical droplets (Langmuir and Blodgett 1949) as

$$C_D = \frac{24}{\mathrm{Re}}\left[1 + 0.197\,\mathrm{Re}^{0.63} + 0.00026\,\mathrm{Re}^{1.38}\right] \tag{4.4}$$

where

$$\mathrm{Re} = \frac{\rho_a D |U_i - V_i|}{\mu_a} \tag{4.5}$$

is the Reynolds number and μ_a is the viscosity of air. The relaxation time τ_p defined in Equation (4.3) has physical significance with regard to dispersion, in that it is the e-folding time required for a droplet to catch up to its local velocity (for V_i to approach U_i).

With a specification of the local velocity field U_i, Equations (4.1) and (4.2) can be solved to obtain the mean trajectory paths for the spray material from each nozzle. Reed (1953) assumed that a counter-rotating pair of vortices, positioned at the aircraft wingtips, generated the local velocity field. This velocity field provides most of the velocity effects close to the aircraft, and will be described later.

Substitution of Equations (4.1) and (4.2) into the full Lagrangian equations results in ensemble-averaged fluctuation equations of the form

$$\frac{d}{dt}\langle x_i x_i \rangle = 2\langle x_i v_i \rangle \tag{4.6}$$

$$\frac{d}{dt}\langle x_i v_i \rangle = \left[\langle x_i u_i \rangle - \langle x_i v_i \rangle\right]\left[\frac{1}{\tau_p}\right] + \langle v_i v_i \rangle \tag{4.7}$$

$$\frac{d}{dt}\langle v_i v_i \rangle = 2\left[\langle u_i v_i \rangle - \langle v_i v_i \rangle\right]\left[\frac{1}{\tau_p}\right] \tag{4.8}$$

where u_i is the fluctuating local velocity. Equation (4.6) represents the growth of the spray cloud, as $\langle x_i x_i \rangle$ is the position variance around the mean droplet location X_i. Equations (4.7) and (4.8) require the specification of $\langle x_i u_i \rangle$ and $\langle u_i v_i \rangle$, correlations of the droplet position and velocity with the local background velocity, respectively, before solution is possible. This development is detailed in Teske et al. (2003) and involves use of a Lagrangian spectral density function determined by von Karman and Howarth (1938) and Houbolt et al. (1964).

With the position and velocity information available for the droplet at any time during the simulation, Equations (4.1) and (4.2), and (4.6) to (4.8), may be integrated exactly as an initial value problem for the solution at the next time step, with the assumption that the background conditions U_i, $\langle x_i u_i \rangle$, and $\langle u_i v_i \rangle$ are constant across each time step. The solution may then be advanced one analytical time step at a time for each droplet in the Lagrangian simulation.

4.2 Evaporation

The evaporation model in AGDISP is based on the well-known D-squared law (Trayford and Welch 1977), in which the time rate of change of droplet diameter is taken as

$$\frac{dD}{dt} = -\frac{D}{2\tau_e\left(1-\dfrac{t}{\tau_e}\right)} \tag{4.9}$$

where

$$\tau_e = \frac{D^2}{\lambda_\infty \Delta\Theta\left(1+0.27\,\mathrm{Re}^{1/2}\right)} \tag{4.10}$$

is the evaporation time scale of the droplet, λ_∞ is the evaporation rate, and $\Delta\Theta$ is the wet bulb temperature depression. For water Trayford and Welch (1977) suggested an evaporation rate of $\lambda_\infty = 84.76\ \mu\mathrm{m}^2/(\mathrm{sec}\cdot{}^\circ\mathrm{C})$. Later tests showed that the evaporation rate could be somewhat lower, down to $\lambda_\infty = 70.24\ \mu\mathrm{m}^2/(\mathrm{sec}\cdot{}^\circ\mathrm{C})$ for deionized water (Riley et al. 1995), and that the evaporation rate is further reduced as the relative velocity $|U_i - V_i|$ approaches zero (Teske et al. 1998a).

In AGDISP the active fraction of an individual droplet changes as the droplet evaporates. Evaporation effects are included from both the active and additive ingredients, as well as the carrier, at a single rate of evaporation, applicable for all three components of the spray mix.

4.3 Flow Field Modeling

The behavior of released droplets is intimately connected to the local background mean velocity U_i and turbulence field q^2 through which the spray material is transported. In AGDISP, these local effects are approximated by models for the aircraft and the atmosphere.

4.3.1 Fixed-Wing Rolled-Up Tip Vortices

When an aircraft flies at constant altitude and speed, the aerodynamic lift generated by the lifting surfaces of the aircraft equals the aircraft weight. The majority of the lift is carried by the wings, and generates one or more pairs of swirling masses of air (vortices) downstream of the aircraft. If the rollup of this trailing vorticity can be approximated as occurring immediately downstream of the wing, then the local swirl velocity V_s around each vortex (one on each wing tip) may be given by

$$V_s = \frac{\Gamma}{2\pi} \frac{r}{\max(r, r_c)^2} \tag{4.11}$$

where Γ is the vortex circulation strength

$$\Gamma = \frac{2}{\pi} \frac{W}{\rho_a s U_\infty} \tag{4.12}$$

r is the distance from the vortex center to the droplet, r_c is the vortex core radius, W is the aircraft weight, s is the aircraft semispan, and U_∞ is the aircraft speed. For a vortex pair the superimposed effects of four vortices are used to simulate the overall proximity to the ground, with image vortices maintaining the no-flow inviscid ground condition. The vortex strength Γ decays with time because of atmospheric turbulence, following a simple decay model

$$\Gamma = \Gamma_i \exp\left(-\frac{\mathrm{bqt}}{\mathrm{s}} \right) \tag{4.13}$$

where Γ_i is the initial vortex circulation strength. This functional dependence was validated in a series of aircraft flyovers past instrumented towers (Teske et al. 1993), with an average value of bq = 0.56 m/s for in-ground effect. Out of ground effect, the vortical decay may be approximated by bq = 0.15 m/s, and smoothly transitioned to the surface (Teske and Thistle 2003).

4.3.2 Helicopter in Forward Flight

The helicopter model partitions the helicopter weight between hover downwash and rotor tip vortices as a function of time. The hover downwash model is taken from actuator disk theory for a propeller (Bramwell 1976) and may be written as

$$w_d = \frac{1}{R}\sqrt{\frac{FW}{2\pi\rho_a}} \tag{4.14}$$

where w_d is the downwash velocity at the helicopter rotor plane and R is the rotor radius of the helicopter. The strength of the vortex pair may be found from

$$\Gamma = \frac{2(1-F)W}{\pi\rho_a R U_\infty} \tag{4.15}$$

where F = exp (- x/R) found by matching the behavior of this simple model with detailed helicopter models (Wachspress et al. 2003) as a function of the axial distance x. At the beginning of the calculation x = 0, F = 0, and all of the weight of the helicopter provides downwash through the helicopter rotor blades. As the calculation proceeds, x > 0, $F \rightarrow 0$, and all of the weight transitions to provide vortex motion are identical to that of a fixed-wing aircraft. Because of the exponential decay, the transition between downwash and vortex motion occurs within two rotor diameters behind the helicopter.

4.3.3 Mean Crosswind

In a neutral atmospheric surface layer the lateral velocity V is assumed to follow a logarithmic profile

$$V = V_r \frac{\ln((z+z_o)/z_o)}{\ln((z_r+z_o)/z_o)} \tag{4.16}$$

where V_r is the lateral velocity at the reference height z_r, z is vertical distance, and z_o is surface roughness. With a linear integral scale of turbulence ($\Lambda = 0.65z$), the turbulence level (Donaldson 1973; Lewellen 1977) becomes

$$q_{wind}^2 = 0.845\left[\frac{V_r}{\ln((z_r+z_o)/z_o)}\right]^2 \tag{4.17}$$

Flow effects are additive from all of these contributions to assemble the local velocity U_i and turbulence q^2. Droplet trajectories are followed from their release points at the nozzle locations until they deposit on the surface or move beyond a downwind location where they are no longer computed.

4.4 Canopy Modeling

AGDISP includes an optical canopy model that can be used to remove spray material by impaction upon its vegetation. The probability that a droplet will penetrate a canopy depends upon the total number and size of vegetative elements encountered on its trajectory through the canopy. If the orientation of these elements is assumed to be random, then the probability of penetration for a given path length will be the same in all directions. Here, the probability of penetration P_p is defined as the probability that a droplet traveling along its trajectory will penetrate a typical single tree envelope. The value of P_p is determined from optical measurements as a function of sun incidence angle. Since probability of penetration is a "sunlight" feature, it must be corrected for droplet mass through the collection efficiency of a vegetative element of a given size. What this step implies is that, while probability of penetration may only take on values between 0 and 1, a value of 0 does not guarantee that the canopy will capture all of the droplets traveling through it (although a value of 1 does guarantee that the canopy will not capture any droplets).

In AGDISP it is assumed that the Lagrangian trajectory analysis is not affected by the presence of the canopy. While evaporation changes the drop size distribution without changing the amount of active material in the spray, droplet interception with the canopy changes both.

The canopy is divided into layers. It may be argued that the probability that sunlight will penetrate one tree layer can be written as

$$P_k = \exp(-\Delta LAI_k) \tag{4.18}$$

where ΔLAI_k is the incremental Leaf Area Index across the incremental canopy height Δz_k, and only vertical measurement of LAI through the height of the canopy is assumed (Teske and Thistle 2004b). The overall probability of a droplet penetrating a tree layer is then given by

$$P_{Tk} = 1 - E\,(1 - P_k) \tag{4.19}$$

where E is the collection efficiency of the vegetative elements comprising the trees, and is determined by impaction with various representations of tree vegetative elements (May and Clifford 1967). Probabilities multiply through the canopy layers.

4.5 Deposition Modeling

Deposition begins as released spray material approaches the ground, continuing until all unevaporated material is deposited. Ground deposition is computed by assuming that the concentration of material around the mean may be taken as Gaussian

$$C = \frac{1}{2\pi\sigma^2}\exp\left[-\frac{(y-Y)^2}{2\sigma^2}\right]\exp\left[-\frac{(z-Z)^2}{2\sigma^2}\right] \tag{4.20}$$

where the released spray material is at position (Y, Z). When the unevaporated material deposits as it approaches the surface, Equation (4.20) is integrated to give

$$M = \frac{1}{2\sqrt{2\pi}\sigma}\exp\left[-\frac{(y-Y)^2}{2\sigma^2}\right]erfc\left(\frac{Z}{\sqrt{2}\sigma}\right) \tag{4.21}$$

Deposition to the ground is estimated by summing all incremental contributions to M as integration proceeds, then correcting the integrated deposition so that conservation of the released nonvolatile spray material is achieved. It may be seen that for material falling vertically toward the surface, the pattern of chemical deposition to the ground generated by Equation (4.21) will be identical to the traditional Gaussian deposition pattern.

5 Conclusions

Techniques for modeling pesticide spray deposition from a boom ground sprayer and an agricultural spray aircraft have been presented. The models shown are mechanistic, design decisions being generally driven by the desire to have an applied model that can be used in regulatory applications. The assemblages of equations shown above generally have highest accuracy when considering the landing position of large drops near the release point. Accuracy generally decreases when smaller droplets and longer downwind distances are considered, plus the models shown use single point meteorology that limits the downwind domain of these models. Current work is focusing on the incorporation of more realistic meteorological approaches that will allow multiple point meteorology to be used. Of course, these approaches greatly increase the complexity and input requirements of this modeling.

Since much of the model development has been driven by regulatory concerns, the assumption that unintended environmental consequences are greater from aerial spraying drove the aerial spray modeling to a level of sophistication (at least in the regulatory domain) ahead of the ground sprayer modeling. The scrutiny aerial spraying has been put under (including the physical understanding gleaned through the model development process) has led to changes in equipment and practice that have greatly improved the environmental footprint of aerial spraying. Attention is now focusing on advancing the state of the art in modeling ground spraying. This is leading to exciting work in this field that is ongoing. Among current questions relevant to both modeling approaches are such issues as the degree to which droplet cloud effects impact landing position and more sophisticated approaches to the handling of lateral obstacles and canopies.

As food and fiber production need to expand to meet the needs of a growing population, the understanding of the pesticide application process continues to be a critical need. As the increasing human population puts more stress on the natural environment, minimizing unintended consequences of pesticide application is also crucial. It is hoped that the increased understanding gained from the development of the models described here as well as the availability of these modeling tools, will aid in achieving both of these goals.

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