IDEFICS: a physical model of spray drift from boom sprayers in agriculture

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ABSTRACT

A random-walk model, IDEFICS, is developed to describe downwind spray deposits from a conventional boom sprayer for chemical crop protection in agriculture. Cumulative spray deposits from a large number of individual drops are calculated downwind from the sprayed crop. The model basically is two-dimensional (2D), but near the nozzle a 3D approach is necessary, to incorporate driving speed and entrained air flow. The model was calibrated with a set of single-nozzle outdoor experiments in a cross wind, with varying nozzle type, liquid pressure, boom height, and driving speed. Weather conditions were measured at the site. The drop size spectrum of the nozzles as well as drop velocity distribution were measured with phase-Doppler anemometry (PDA). Both experiments and model results showed that boom height, average wind speed and nozzle type were the major factors affecting spray drift. The IDEFICS model appears to be a useful tool to investigate spray drift under varying conditions.

NOTATION

a, b, c	constants describing drag coefficient	q	lateral distance from spray cone axis
C_d	drag coefficient	Re	Reynolds' number
d_r	roughness length (ca. 0.1 z_c)	r, s	constants in rate of evaporation
d_z	zero plane displacement (ca. 0.7 z_c)	t	time
D	drop diameter	Δt	time step
f_h, f_{ph}	constants related with entrained air flow	$u, \vec{u}$	velocity of air
$\vec{g}$	gravitational acceleration vector	u_*	friction velocity
h	distance below spray nozzle	$v, \vec{v}$	velocity of spray drop
h_{sh}	length of liquid sheet	v_0	liquid velocity at nozzle outlet
k	Von Karman's constant (ca. 0.41)	$\vec{x}$	position vector of spray drop
K	constant related with crop structure	z	distance above ground level
K_e	rate of decay of entrained air velocity	z_c	crop height
p	distance from spray cone axis		
α	$= \exp(\beta)$	τ	relaxation time of droplet
β	$= \Delta t/\tau$	φ, ψ, ζ	local variables defined in this paper
ρ	mass density		

Subscripts

A	referring to air	i	time step number
ax	referring to axis of the spray cone	L	referring to spray liquid
c	referring to crop height	p	referring to p-direction (entrained air)
e	referring to entrained air	s	referring to sedimentation
h	referring to h-direction (entrained air)		

INTRODUCTION

In agriculture, chemical crop protection is still inevitable. However, unlimited use of pesticides may severely endanger the environment and human health. In the Netherlands, the reduction of pesticide use and danger is based on three goals (1):

- reduction of dependence on pesticides;
- reduction of the amount of pesticides used;
- reduction of emission and drift of pesticides.

Contamination of surface water and ditches surrounding crop fields has gained special attention. Investigating emission and drift of pesticides in field experiments is very laborious. Assessing the effect of a single parameter is hard due to the fact that many parameters change simultaneously, unless a large number of independent experiments is carried out. This makes the development and use of a computer model to estimate spray drift and downwind deposits worthwhile. The IDEFICS spray drift model (IMAG program for Drift Evaluation for Field sprayers by Computer Simulation) was developed to be complementary to field experiments and to estimate spray drift in practical applications (2).

CONCEPTUAL MODEL DESCRIPTION

The IDEFICS spray drift model is a mixed 2-3-dimensional (2D/3D) random-walk model, which describes the trajectories of a large number of individual drops produced by a single nozzle (see Fig 1). A complete boom sprayer is simulated by repeating these calculations for a representative set of nozzles along the boom. The distribution of downwind deposits in a cross wind is calculated as a function of distance from the edge of the crop. The vertical distribution, at a fixed distance downwind, is calculated as well. Optionally the model can be provided with a V-shaped ditch parallel to the crop edge.

Integrating twice Newton's second law of mechanics, the position of a drop can be calculated. The forces experienced by a drop are gravity, buoyancy and drag force due to local air velocity relative to the velocity of the drop itself. Gravity is calculated straightforward, and buoyancy can be neglected completely in this case. The drag force however changes continuously, since most parameters involved change with respect to location in space.

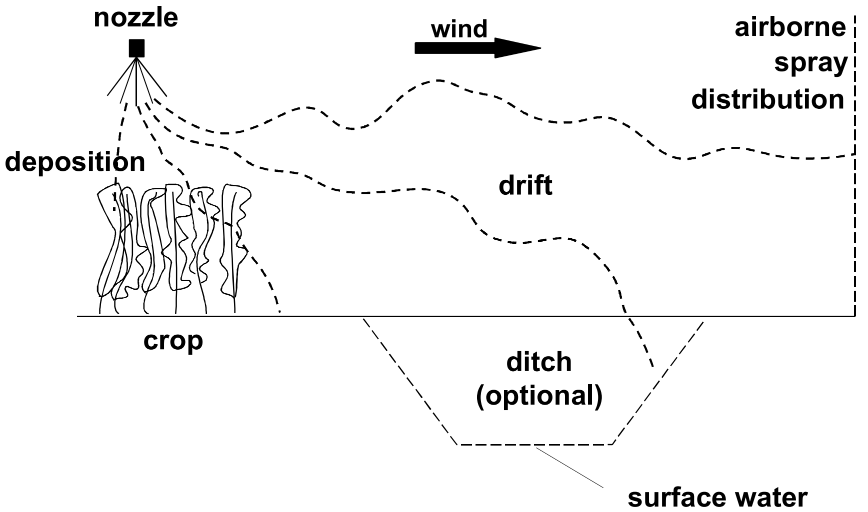

Fig 1. Typical field lay-out for the simulation model.

Therefore the integration procedure must take place stepwise in time. During a certain time interval all parameters are considered constant. At the end of each interval all parameters are recalculated depending on the local conditions. The time interval must be short near to the nozzle, but can be longer at some distance from the nozzle. Therefore the optimal time interval should change according to local conditions too. In the model the time interval is estimated based on the expected rate of change of the relaxation time of the drop.

In the spray cone below the nozzle air is entrained, which causes small drops to flow downward much more rapidly than estimated with respect to their sedimentation velocity. Modelling the spatial distribution of entrained air velocity and direction appropriately is considered an important base for a correct estimate of spray drift. Phase-Doppler anemometry (PDA) is used to measure the distribution of drop size and velocity in the spray cone. Entrainment is affected by wind speed, driving speed and the vicinity of the ground. In IDEFICS, the entrained air flow is modelled empirically based on the PDA measurements and patternator experiments. The effect of the vicinity of the ground, which obviously is impenetrable to air, is modelled by introducing an imaginary upward spraying nozzle below ground level. The entrained air flow caused by the imaginary nozzle is added to that caused by the real nozzle.

Near the nozzle the trajectory calculations are 3D. At a certain distance from the nozzle entrainment and driving speed no longer affect the trajectory, and the process essentially becomes 2D, so calculations can be turned into 2D.

The average wind velocity is assumed logarithmic with height above the ground, following the widely used meteorological relation (3). Turbulence is added as a locally random air velocity, its strength depending on local average wind velocity and atmospheric stability. The turbulence velocity vector has random direction, and its length represents intensity. Inside the crop the wind profile has to be adjusted (3).

While falling or drifting through air, drop size decreases due to evaporation. It is assumed that only water evaporates as if the drop was of pure water. The ingredients are essentially involatile during spraying. This is known as the 'solid-core' phenomenon (4). If all water is lost before settling, the remaining 'dry' particle is assumed to stay airborne throughout.

MATHEMATICAL STRUCTURE

Basic equations

The calculation of the trajectory of a spray drop in air is described by Newton's second law of mechanics (the well-known *F=ma*), and integrating it twice. Assuming that the various forces acting on the drop can be considered constant during time interval Δt, velocity and position of the drop at time i+1 are given by:

$$\vec{v}_{i+1} = \vec{v}_i\,\alpha_i + \vec{v}_{s,i}\left(1-\alpha_i\right) \qquad [1]$$

$$\vec{x}_{i+1} = \vec{x}_i + \vec{v}_i\,\Delta t + \tau_i\left(\vec{v}_{s,i} - \vec{v}_i\right)\left(\alpha_i - 1 + \beta_i\right) \qquad [2]$$

For convenience the terms α_i and β_i are introduced. All quantities are essentially time dependent and therefore suffixed i. From now on, for clarity the suffix i will be omitted. The equations given are exact solutions, as long as the quantities $\vec{v}_s$ and τ (and consequently α and β) remain constant at Δt. The sedimentation velocity $\vec{v}_s$ depends on gravity and local wind velocity:

$$\vec{v}_s = \tau\,\vec{g} + \vec{u} \qquad [3]$$

where the first term equals the vertical component of sedimentation due to gravity, and the second term represents the effect of local wind velocity. This local wind velocity comprises average wind velocity and random wind velocity due to air turbulence, both being local parameters.

Derivation of optimal time interval

The relaxation time τ represents the time a drop needs to adapt to changes in local air flow, and is given by:

$$\tau = \frac{4\rho_L D}{3\rho_A v_r C_d} \qquad [4]$$

The drag coefficient C_d for a solid spherical particle in air is very well described by the empirical relation:

$$C_d = \left(\left(\frac{a}{Re}\right)^c + b^c\right)^{1/c} \qquad [5]$$

with constants a=24, b=0.32 and c=0.52. This relation fits very well to experimental data (5) for Reynolds' numbers up to 10^4, which is far beyond values occurring in conventional spray applications.

In all practical cases the time step Δt is limited much more by the rate of change of τ than by that of $\vec{v}_s$. This means that the time step can be derived from the allowable ratio $|\Delta\tau/\tau|$. This ratio can be estimated by taking the derivative of τ. Since [4] essentially is a function of v_r and D, which both can be considered functions of time themselves, the following equation results:

$$\Delta\tau = \frac{\partial\tau}{\partial v_r}\frac{dv_r}{dt}\Delta t + \frac{\partial\tau}{\partial D}\frac{dD}{dt}\Delta t \qquad [6]$$

The first term represents the change in τ due to changes in drop velocity, local air velocity or their directions. The second term represents the effect of evaporation on τ.

The rate of evaporation of water drops in air is described by Williamson and Threadgill (6). Since only medium to small sized drops spend long enough time in air to be affected by evaporation, and noting that their time of flight usually is much longer than their relaxation time, it is reasonable to assume that the velocity of a drop is close to its sedimentation velocity, as far as evaporation is considered. Then the rate of evaporation of a drop falling through air is simplified considerably:

$$\frac{d(D^2)}{dt} = rD + s \qquad [7]$$

where r and s are constants depending on temperature and humidity.

Finally, from (6) the limitation for the time step Δt is derived:

$$\Delta t \le \frac{1}{\zeta}\left(|\Delta\tau/\tau| - \frac{\varphi}{1+\psi}\right) + \frac{\varphi}{\zeta\left(1+\psi\right)}\,exp\left(-\Delta t/\tau\right) \qquad [8]$$

where the following abbreviations are used:

$$\varphi = \frac{\left|\vec{v}_s - \vec{v}\right|}{v_r} \qquad \psi = \left(\frac{a}{b\,Re}\right)^c \qquad \zeta = \frac{2\psi+1}{\psi+1}\,\frac{\left|rD+s\right|}{2D^2} \qquad [9]$$

Given an acceptable relative change in relaxation time, $|\Delta\tau/\tau|$, the maximum time step is estimated by [8]. Clearly [8] must be solved iteratively. If the initial guess of Δt is appropriate, usually only a small number of iterations is required.

Wind profile

The average wind velocity is assumed to be logarithmic with height, according to the following the meteorological equation:

$$u(z) = \frac{u_*}{k} \, ln\left(\frac{z - d_z}{d_r}\right) \qquad [10]$$

Zero plane displacement d_z and roughness length d_r are roughly proportional to crop height (7). Air turbulence is quantified by the turbulent exchange coefficient (eddy diffusivity), which depends on average wind velocity and atmospheric stability.

Inside the crop canopy the logarithmic profile has to be replaced by the equation:

$$u(z) = \frac{u_c}{\left(1 + K\left(1 - z / z_c\right)\right)^2} \qquad [11]$$

where u_c is the average wind velocity at crop height z_c. Constant K depends on crop structure, and is roughly equal to 2 (3).

Entrained air flow

Following the relation of Briffa and Dombrowski (8), the velocity of entrained air at the axis of the spray cone is given by:

$$u_{e,ax}(h) = v_0 \left(\frac{h_{sh}}{h}\right)^{K_e} \qquad [12]$$

For various types of flat fan nozzles the rate of decay K_e appears to be approximately equal to 0.7. The liquid sheet length h_{sh} is estimated from comparison of [12] and PDA measurements, and varies roughly between 10-20 mm.

In a plane perpendicular to the axis of the spray cone, the velocity of entrained air is modelled by:

$$v_e(p,q,h) = v_{e,ax} \cdot \frac{1}{4}\left[cos\left(\frac{\pi p}{f_h p_0}\right) + 1\right]\left[cos\left(\frac{\pi q}{f_h q_0}\right) + 1\right] \qquad [13]$$

where p and q represent the two orthogonal distances from the cone axis, in the two main directions of the elliptic cone. Their geometrical limits are p_0 and q_0, which depend on top angle and 'lateral' top angle respectively, and on distance h below the nozzle outlet. Constant f_h is an extension factor to account for entrained air flow outside the geometrical limits of the spray cone, and is empirically set between 1.2 and 1.8.

Equation [13] gives the velocity amplitude of a velocity which essentially is 3D. Since the lateral top angle is usually relatively small for flat fan nozzles, the component of the entrained air flow in the lateral horizontal direction (q-direction) is neglected.

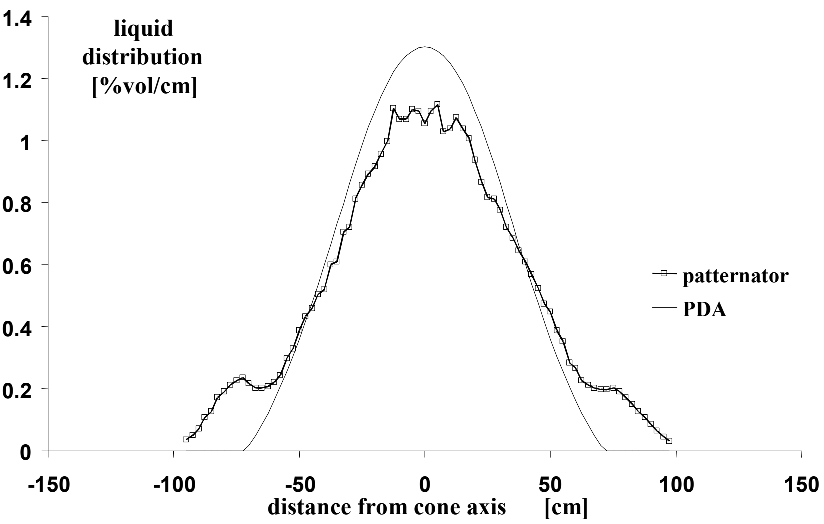

Fig 2. Distribution of spray liquid below a flat fan nozzle (F, 0.8L/min@300kPa) as deposited on a patternator and in air (PDA), as measured 0.5m below the nozzle. The side-wings in the patternator experiment account for the 'ground effect'.

This leaves the air flow 2D: a horizontal component (p-direction) and a vertical component (h-direction). Their ratio is assumed to be given by:

$$\frac{v_{e,p}}{v_{e,h}} = f_{ph} \cdot \frac{p}{h} \qquad [14]$$

Factor f_{ph} represents the deviation of the direction of flow from a straight line back to the nozzle outlet, and is empirically set to 0.9.

Obviously the ground is impenetrable to air flow, and the air flow due to entrainment must deviate close to the ground towards a horizontal air flow. This 'ground effect' is modelled by introducing an 'image concept': an imaginary subsoil nozzle spraying upward induces an air flow which is the mirror of the air flow caused by the real nozzle. As a result, in the plane just in the middle of these two nozzles the resultant velocity is horizontal. The image concept is slightly modified based on patternator experiments with a stationary nozzle. Fig 2 shows the spreading effect caused by the vicinity of an impenetrable surface.

Driving speed and wind velocity will affect entrainment. In a first approach it is assumed that the entrained air flow is merely shifted sideward in a horizontal plane.

CALIBRATION EXPERIMENTS

Experimental setup

Calibration experiments were carried out using an experimental single-nozzle spraying carriage. The carriage was pulled at constant speed over a 15m track, the track being placed perpendicular to average wind direction. All experiments were carried out on a field of cut grass (height ca. 0.05 m). The experiments included various boom heights, nozzle types, liquid pressures and driving speeds. The weather conditions were recorded. The spray liquid was tap water containing fluorescent dye (1.0g/L Brilliant Sulfoflavin, BSF) and a surfactant (1mL/L Agral™). Spray deposits on the ground were measured up to 5m downwind, using synthetic cloths as collectors. The amount of spray drops still airborne at 5m downwind was measured using a vertical pole supplied with synthetic spherical collectors (diameter 0.08m), up to 2.5m above the ground.

The experiments include four boom heights (0.35, 0.50, 0.75 and 1.00m above cut grass), four driving speeds (0.1, 0.25, 1.0 and 1.5m/s), three flat fan nozzles (top angle 110^{o}, BCPC size classes fine (F; 0.8L/min@300kPa), medium (M; 1.6L/min@300kPa), and coarse (C; 3.2L/min@300kPa). A detailed description of the experiments and the results is given elsewhere (2).

Drop size spectra were measured using PDA technique (Aerometrics' Phase-Doppler Particle Analyzer). The nozzle was moved slowly across the laser beams to obtain a size distribution averaged over the whole spray cone. Sprays were scanned 0.5m below the nozzle. The velocity of the drops were measured at the centreline of the spray cone.

Results

Experimental ground deposits were compared with results from simulations. Fig 3 shows an overall plot of these deposits. For deposits above 10% of the applied dosage the measured and calculated deposits agree very well. For lower deposits the calculated results overestimate the actual deposits, up to a factor 2-3 below 1% of the applied dosage. After calibration of the model results, using regression analysis, the calculated and measured deposits agree reasonably well on average. The spread of data, however, has not decreased. Apparently there is some random deviation not accounted for yet. Local fluctuation of wind direction may be the most important. On the other hand, the measuring accuracy of deposits below 0.1% of the applied dosage is low.

CONCLUSION

The IDEFICS spray drift model is a useful tool to obtain data on spray drift from conventional agricultural boom sprayers. Drop size distribution as well as entrained air flow is directly based on actual measurements with PDA technique. The calibrated model can estimate actual downwind spray deposits well on average, though coincidental spreading occurs for individual measurements.

Future calibration experiments will be used to increase the accuracy of the model and to extend its range of use to other conditions, such as other nozzle types, the presence of a crop.

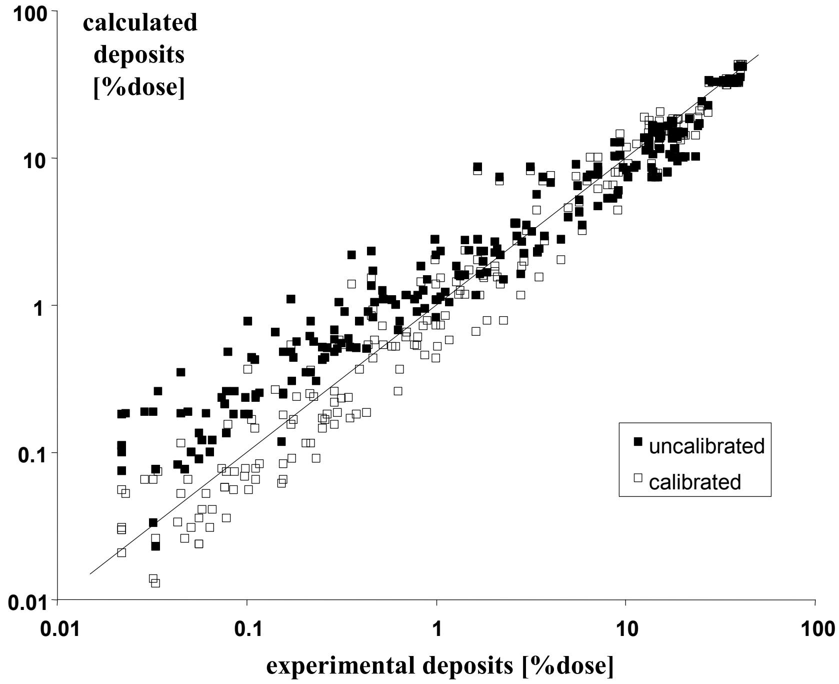

Fig 3. Correlation between measured and calculated deposits, before and after calibration. The solid shows the ideal relationship (y=x).

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