GEOMATICS AND ENVIRONMENTAL ENGINEERING • Volume 19 • Number 5 • 2025

https://doi.org/10.7494/geom.2025.19.5.23

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DRIMERA: New Model of Airborne Pesticide Dispersion by Eulerian Approach Coupled with Weibull's Law and Wind Rose

Abstract: To solve the constraints that are commonly faced in risk assessment, research on the modeling of the dispersion and distribution of pollutants in the environment are emerging, and software is being developed. This paper presents a tool that is based on the Eulerian approach coupled with Weibull's law and the wind rose approach (called DRIMERA). This physically detailed modeling-based software can accurately predict pesticide drift under different weather conditions and calculate aerially applied pesticide concentrations in the environment at a threshold of $p = 0.05$; the values of the coefficient of determination r^2 vary between 0.6331 and 0.9876. This support thus helps facilitate the wider use and adaptation of atmospheric models.

Keywords: modeling, software, DRIMERA, risk assessment, pollutant dispersion

Received: May 28, 2024; accepted: July 3, 2025

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1. Introduction

According to the United Nations Environment Program (UNEP) [1], pesticides cause nearly 385 million cases of accidental non-fatal poisonings annually; among the approximately 2 million annual cases of pesticide-related deaths, 8 to 17 percent of these victims die from self-poisoning. Several cases of cancer, childhood leukemia, and certain effects on the neurological, immunological, and reproductive systems are linked to occupational or residential exposure to pesticides [1]; thus, human health preservation and environmental protection against pesticides has become essential. Moreover, these are the two major concerns in risk assessment [2]. In this process, exposure assessment (which is a step that can be treated at the same time as hazard characterization) is used to establish the objective conditions of the exposure to the target organisms [3]. Exposure to pesticides depends on both exposure hypothesis and pesticide concentration; these can be determined in the different compartments of the environment – either from measurement or modeling.

The concentration modeling of contaminants such as pesticides in the environment is part of a more general framework of indirect risk analysis. This permits us to solve the constraints that are commonly faced in risk assessment by the availability of measurement data; these are the large amount of data to be measured, short collection times, insufficient data (even when available), and the absence of the bioaccumulation of the pollutant in the target organism [4]. In the context of an indirect approach to exposure assessment, organizations such as America's Environmental Protection Agency (EPA) and the World Health Organization (WHO) recommend the use of scientifically recognized analytical methods to ensure the reliability of any results [5]. The current scientific literature is, thus, abundant in studies on subjects as varied as the statistical analysis of environmental data [6–9], pollutant-dispersion modeling [10–13], measurement techniques in biological and inert media [14–16], cell-level-effect modeling [17], and methods for quantifying uncertainties in results [18–20]. In this regard, several studies have successfully used pesticide-dispersion modeling to assess risks [21–23]. This is also the case for the model of the German Biological Research Centre for Agriculture and Forestry (BBA), which has been indispensable in the context of the risk assessment of surface water pollution [24, 25]. At the end of their study, they recommended mitigation measures on the use of safety zones and the application of drift-reduction techniques. In addition, the model that was developed by the EPA and is commonly used in the United States and Canada remains an important tool in the risk assessment of phytosanitary treatments. Another study on modeling as part of the assessment of the potential risks of pesticide exposure of organisms that was carried out by Ganzelmeier et al. [26] resulted in a tool for proposing a safety zone around an agricultural plot. The model that was developed in this case was based on drift-measurement campaigns during the phytosanitary treatments of crops. In view of these results, the modeling of pesticide concentrations can be used to assess the risks that are associated with phytosanitary treatments in banana plantations.

In this paper, we present the new DRIMERA model: user-friendly graphical interface (GUI) software that is based on the Euler approach for determining aerially applied pesticide concentrations in the environment. It aims to assess the risk that occurs in such cases as in the aerial treatment black leaf streak disease (BLSD) in bananas.

2. Methodology

2.1. DRIMERA Tool Description

Workflow

DRIMERA, which stands for "drift modeling for environmental risk assessment," is a decision-support tool. Developed with Python programming language, this software is a dual-model for airflow forecasting and pesticide droplets distribution that, based on the phytosanitary treatment conditions of crops by aerial spraying (meteorological and operational data), simulates the dispersions of pesticides in the environment as concentration values. Allowing for a simulation of the atmospheric dispersions of pollutants, it thus helps to evaluate the risks that are related to the use of pesticides by air on crops such as banana plantations. The conceptual scheme of the DRIMERA pesticide-dispersion model is shown in Figure 1.

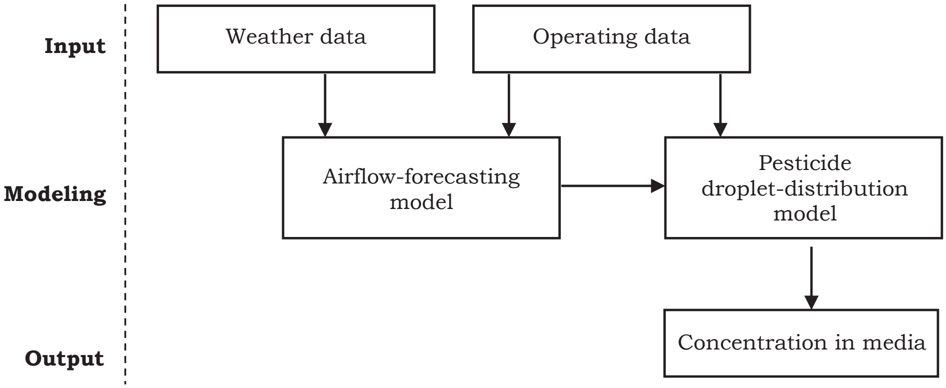


Fig. 1. Conceptual scheme of DRIMERA pesticide-dispersion model

DRIMERA is based on the following assumptions:

- wind speed is 2D (vertical component z is null);
- air flow varies in time and space;
- droplet-ejection velocity is vertical and constant for all diameter classes [27];
- only water contained in carrier liquid is lost to air, resulting in decrease in diameter and increase in droplet concentration; when diameter becomes zero, pesticide has completely sublimated [28, 29].

On this basis, the calculations proceed as follows:

- Step 1: reconstitution of particle-size spectrum and calculation by diameter class, volume fraction, droplet number, and cumulative volume fraction;
- Step 2: calculation of air flow;
- Step 3: calculation of sedimentation velocity to determine altitude of droplets;
- Step 4: calculation of dispersion around impact point.

Selection of Parameters

DRIMERA model requires parameterization in terms of meteorological data on the one hand and operational parameters that are related to the spraying aircraft on the other. Table 1 shows this required data.

Table 1. Input data that is required by DRIMERA

Parameter	Description	Unit
Pesticide used	Pesticide to be used during phytosanitary treatment; existing database compiles a list of pesticides currently used in Ivory Coast and Cameroon	–
Pesticide volume	Specifying quantity of liquid pesticide to be used	L
Carrier material	Carrier material to be used for mixture; existing database to be updated is available	–
Carrier volume	Specifying quantity of carrier material to be used	L
Boom height	Spray height above ground	m
Application rate	Quantity of spray that is applied per hectare of field	$L \cdot ha^{-1}$
Nozzle spacing	Distance in two successive nozzles	cm
Spray particle size	Spray droplet characteristics in average diameter d_{50} (fog, very fine, medium, coarse, fine rain) related to nozzle properties and ejection speed	μm
Forward speed	Aircraft overflight speed	$m \cdot s^{-1}$
Ground concentration	Residual concentration of pesticides that are considered to be uniform on ground before spraying	$\mu g \cdot L^{-1}$
Wind speed	Average wind speed in direction of flow considered; parameterization of local wind rose is required; existing database to be updated is available	$m \cdot s^{-1}$
Temperature	Average temperature at time of spraying	°C
Relative humidity	Average relative humidity at time of spraying	%

User Interface

DRIMERA is a friendly useful interface (as is presented in Figure 2), and the user interface (presented in two quadrants) is easy to use. The "Input" quadrant takes the input data that is presented in Table 1 into account. Once the data is implemented, the simulation results are displayed in the "Output" quadrant. The "Output" quadrant components are presented in Table 2.

To make it easier to get started with the software, a "Help" tab is available.

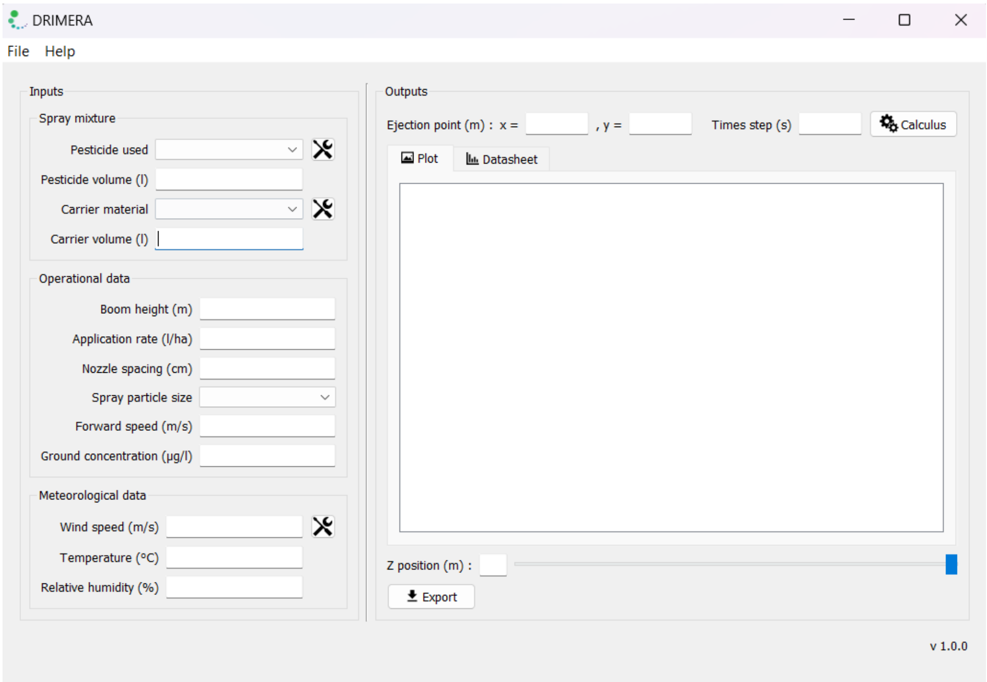


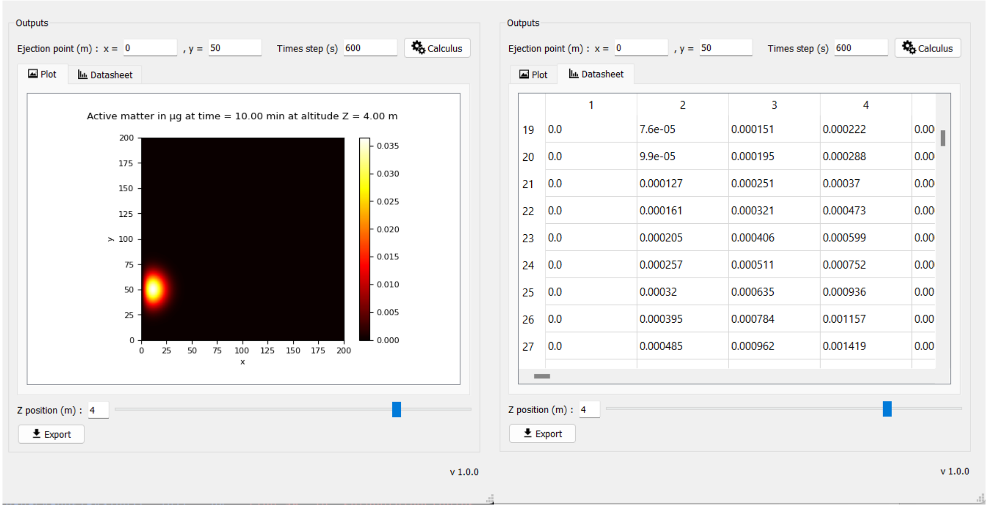
Fig. 2. DRIMERA user interface

Table 2. DRIMERA output components

Component	Description
Ejection point x	x-coordinate in m at initial point of spraying
Ejection point y	y-coordinate in m at initial point of spraying
Time step	Simulation time of pesticide dispersion [s]
Calculus	Starting button of simulation
Plot	Graphic tab that presents simulation results as image; presented values are pesticide's active matter mass in micrograms [µg] dispersed at different altitudes up to ground
Datasheet	Tabular tab that presents simulation results as table; presented values are pesticide's active matter mass in microgram [µg] dispersed at different altitudes up to ground
z position	Defining z-coordinate in m to visualize pesticide's active matter mass distribution at different altitudes (from ground to boom height)
Export	Button to download results by format depending on chosen tab

Result Display

After entering the calculation time "Time step" and starting the simulation with the "Calculus" button, the results of the simulation are presented in the "Plot" tab graphically on the one hand and in the form of a data table in the "Datasheet" tab on the other (Fig. 3). These results are obtained as active matter quantity values of the pesticide (expressed in micrograms [µg]) in the environment. The different quantity values are obtained at "*z* position," varying from the ground (*z* = 0) to the boom height from the *x* and *y* ejection position. The "Export" button also allows one to download the obtained results in each tab.



Ejection point (m) : x = 0 , y = 50

Times step (s) 600

Z position (m) : 4

	1	2	3	4	
19	0.0	7.6e-05	0.000151	0.000222	0.00
20	0.0	9.9e-05	0.000195	0.000288	0.00
21	0.0	0.000127	0.000251	0.00037	0.00
22	0.0	0.000161	0.000321	0.000473	0.00
23	0.0	0.000205	0.000406	0.000599	0.00
24	0.0	0.000257	0.000511	0.000752	0.00
25	0.0	0.00032	0.000635	0.000936	0.00
26	0.0	0.000395	0.000784	0.001157	0.00
27	0.0	0.000485	0.000962	0.001419	0.00

Fig. 3. DRIMERA results displayed in graphical and data table tabs

2.2. Models' Descriptions

The basic dispersion model is of the Euler type and was influenced by the physicochemical phenomena of deposition. Indeed, the movement of pesticides spreading in the air and constituting an atmospheric mixture [30] is a multiphase flow where a continuous fluid phase coexists between the air and a dispersed fluid phase (in this case, the pesticide droplets). The latter will be described according to the Eulerian formalism for solving Navier–Stokes equations. Coupled with Weibull's law and the wind rose, we then obtained a two-fluid model: on the one hand, an air-flow-prediction model for the carrier phase; and on the other, a droplet-flow model (Fig. 1).

Airflow Forecasting

Different methods enable the modeling of wind-speed distribution; however, Weibull's law is the most commonly used one [31]. This is a continuous probability law that is characterized by the parameters of shape k (dimensionless) and scale λ [$m \cdot s^{-1}$].

The density function of Weibull’s law is as follows:

$$f(v) = \left(\frac{k}{\lambda}\right)\left(\frac{v}{\lambda}\right)^{k-1} e^{-\left(\frac{v}{\lambda}\right)^{k}} \tag{1}$$

with $f(v)$ being the probability of the occurrence of wind speed v [m·s^{-1}].

The speeds distribution is, thus, obtained with the inverse of Weibull’s law in such a way that:

$$v = \left[-\lambda^{k} \ln(1-X)\right]^{\frac{1}{k}} \tag{2}$$

where X is a uniform law on [0, 1].

The k and λ parameters (obtained from mean speed $\overline{v}$ [m·s^{-1}]) and the standard deviation σ [m·s^{-1}] of a database of wind speeds that are characteristic of the site are determined empirically by Saleh et al. [32]:

$$k = \left(\frac{\sigma}{\overline{v}}\right)^{-1.086} \tag{3}$$

$$\lambda = \frac{\overline{v}}{\Gamma\left(1+\frac{1}{k}\right)} \tag{4}$$

with Γ being the gamma function.

Furthermore, this would only be complete by integrating the wind rose considering the wind speed spatiotemporal variability. Wind rose is a graph that indicates the distribution of the wind direction at a given location over a considerable period of time [33]. Characteristic of a given geographical area, this graph is obtained during an observation period of at least one-month groups together with the frequencies of the directions from which the wind originates and the wind strength frequencies for each wind direction (Fig. 4). The frequencies of the wind occurrence were distributed as a probability of occurrence over 360° and divided into eight sectors of 45°; therefore, they appear as polar coordinates in the forms of distances from the origin that are proportional to the probability that the wind direction is at a given sector.

We thus obtain air-flow-prediction model $V(u_{i,j}^{a}, v_{i,j}^{a})$ for the dispersed phase.

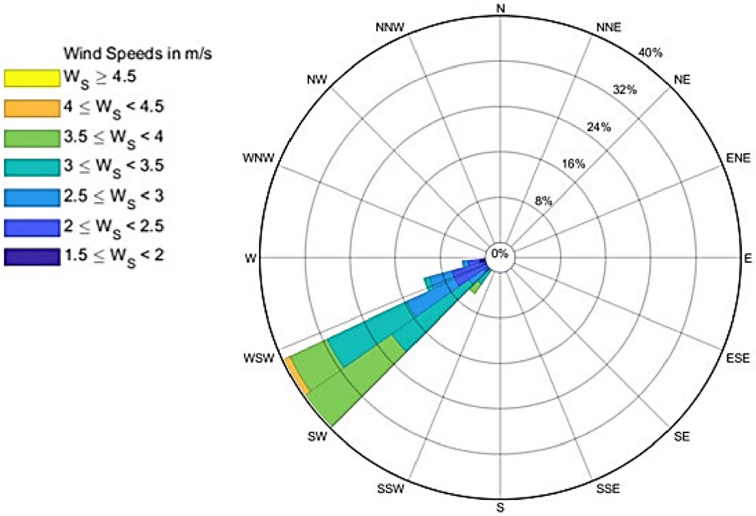


Fig. 4. Wind rose at 10 m in Abidjan, Ivory Coast

Source: [34]

Pesticide Ejection

During aerial spraying, pesticides are ejected from the nozzles in the forms of spherical droplets. The flow of the droplets initially dominated by their inertia and their emission velocity V_0 and are, thus, only affected by that of the air:

$$V_0 = \sqrt{\frac{2\nu_e P}{\rho_l}} \tag{5}$$

with ν_e being the efficiency of the atomization process, P – the pressure at the nozzle outlet [m], and ρ_l – the droplet density [kg·m^{-3}].

According to Cerruto et al. [35] and Privitera et al. [36], the droplets obey the sizes that follow the log-normal distribution (6):

$$f(d) = \frac{1}{\sqrt{2\pi}\, d \ln \sigma_g} \exp\left(-\frac{\left(\ln \frac{d}{d_{50}} \right)^2}{2\ (\ln \sigma_g)^2} \right) \tag{6}$$

where $f(d)$ is the fraction of diameter d, d is the droplet diameter [μm], and d_{50} is the mean diameter [μm].

The mean diameter d_{50} that is directly linked to the nozzle type can also be obtained by the classification in Table 3.

Table 3. Droplet mean-diameter classification

Droplet classification	Diameter [μm]
Very fine	20
Fine	100
Medium	240
Coarse	400
Very coarse	1000

Source: [37]

As pesticide droplets are small in diameter and, therefore, in low concentrations, gravity will move the droplets downward in a sedimentation process, while the wind speed will determine the transport in the vertical plane (according to Thistle [30]). The influence of the dispersed phase on the continuous phase is, thus, neglected, and the flow of the droplets is only affected by that of the air.

Dispersed Phase Equations

The equations that are implemented in the air flow are, therefore, those that are linked to the conservation of the mass and momentum and to the drag force (Stokes' drag law):

$$F_{drag} = 3\pi\mu_{air} d_l (u_{air} - u_l) \tag{7}$$

where F_{drag} is the drag force [kg·m·s^{-2}], μ_{air} – the air dynamic viscosity [kg·m^{-1}·s^{-1}], d_l – the droplet diameter [m], u_{air} – the air speed [m·s^{-1}], and u_l – the droplet speed [m·s^{-1}].

The concentration of droplets that are only affected by the air flow is, thus, determined by the advection-diffusion equation such that:

$$\frac{\partial(\rho_l \phi)}{\partial t} + \nabla \cdot (\rho_l \phi u_{air}) = \nabla \cdot (\rho_l D \nabla \phi) \tag{8}$$

with ρ_l being the droplet density, ϕ – the volume fraction of the droplet, and D – the droplet diffusivity.

Calculations of Concentrations

The finite difference method (FDM) is used for the discretization of partial differential equations [38]. The Navier–Stokes equations are discretized by a left-centered or right-centered scheme for first-order partial derivatives and a centered scheme for second-order partial derivatives.

We then obtain the following system of equations while reorganizing the results for programming purposes:

- updating speed of droplets by that of air:

$$\begin{cases} u^{l}_{i,j} = C_d\, u^{a}_{i,j} + (1 - C_d) u^{l}_{i,j} \\ v^{l}_{i,j} = C_d \cdot v^{a}_{i,j} + (1 - C_d) v^{l}_{i,j} \end{cases} \tag{9}$$

- calculating droplet diffusion:

$$c_{i,j} = \Delta t\, D \left[\frac{c_{i+1,j} - 2c_{i,j} + c_{i-1,j}}{\Delta x^2} + \frac{c_{i,j+1} - 2c_{i,j} + c_{i,j-1}}{\Delta y^2} \right] \tag{10}$$

- calculating droplet advection:

$$c_{i,j} = \Delta t\, u^{l}_{i+1,j} \frac{c_{i+1,j} - c_{i-1,j}}{2\Delta x} + \Delta t\, v^{l}_{i+1,j} \frac{c_{i,j+1} - c_{i,j-1}}{2\Delta y} \tag{11}$$

- determining droplet-sedimentation speed:

$$V_s = \sqrt{\frac{4}{3} \frac{g}{C_d} \frac{\rho_l - \rho_a}{\rho_a} d} \tag{12}$$

Drag coefficient C_d is linked to Reynold number Re by the empirical relationship of spheres that was recommended by Perry et al. [39]:

$$\begin{cases} C_d = \dfrac{24}{\mathrm{Re}} (1 + 0.14\,\mathrm{Re}^{0.70}) \text{ for } \mathrm{Re} \le 1000 \\ C_d = 0.447 \text{ for } \mathrm{Re} > 1000 \end{cases} \tag{13}$$

Initial and Boundaries Conditions

The initial conditions of the velocity field (at $t = 0$) are u, $v = 0$, and the initial concentration is that which is entered by the user. The boundary conditions of the simulation domain are such that, at x, $y = \{0, 201\}$, we have $c = 0$.

2.3. Data Validation

After the development of DRIMERA, this model went through a stage of evaluations that tested the reliability of its simulation results. This phase consisted of comparing the simulated values to data that was collected under the same operational and meteorological conditions.

Data-Collection Sites

According to Tuo et al. [40], black leaf streak disease (BLSD) affects all of the banana plantations in Ivory Coast – with the highest average severity index for the ZAE I agroecological zone in particular. This index of 44.57% reflects the increased use of fungicides for BLSD control. This geographical area includes the BANACOMOE, SIAPA, BANACI, SAKJ, and EGLIN banana plantations, which belong to the sub-prefectures of Bécoueffin, Tiassalé, Taabo, Ayamé, and Azaguié, respectively, in Ivory Coast; these were the subject of the data-collection sites as part of this study (Fig. 5). The choices of these sites (which were also used in the FIRCA [41] study on the impacts of pesticide spraying on banana farms) was guided by the sizes of the plantations and the techniques that were used for treating the plantations (airplane, helicopter, or microlight aircraft). These were, therefore, representative of the various configurations of banana farms, thus making it possible to assess the impacts of aerial pesticide spraying practices on different scales and with different methods. These sites thus offered a relevant panorama for studying the effects of pesticides in a variety of agricultural contexts that ranged from small banana plantations to large intensive farms. Thus, the five Ivorian banana plantations were investigated for their different operational and meteorological conditions for this measurement phase.

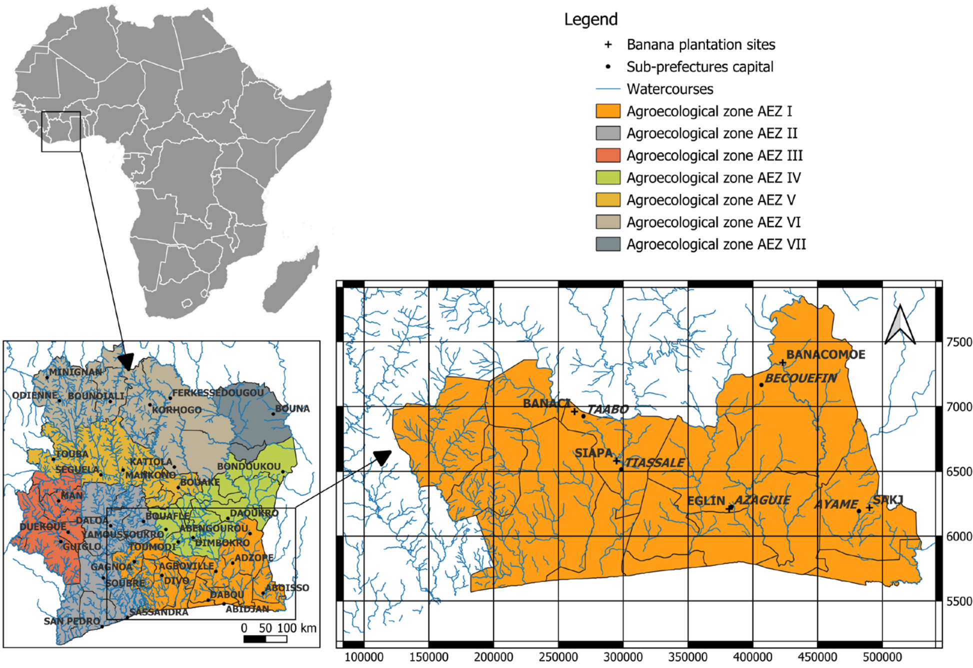


Fig. 5. Map of data-collection sites in AEZ I agroecological zone, Ivory Coast

Drift-Measurement Methodology

Drift data was collected under real land-application conditions according to ISO 22866:2005 [42] during the period of February through March 2018. Indeed, this standard established a standardized methodology for the measurement of drift in the spraying of plant-protection products that are applicable to all types of crop-protection equipment. It precisely defines the parameters to be measured, such as droplet-size distribution, wind speed and direction, temperature, and relative humidity as well as the characteristics of the spray product and the application material.

ISO 22866:2005 [42] also specifies techniques for sample collection (Fig. 6) and analysis as well as field-test conditions, including sensor layout and weather requirements. The aim is to provide comparable and reliable results to assess and quantify drift levels at specific distances (5, 10, 20, 30, 50, and 100 m), thus optimizing the application techniques, reducing the environmental risks, and improving the safety when using plant-protection products. This drift data can also be compared to other data sources such as the DRIMERA tool.

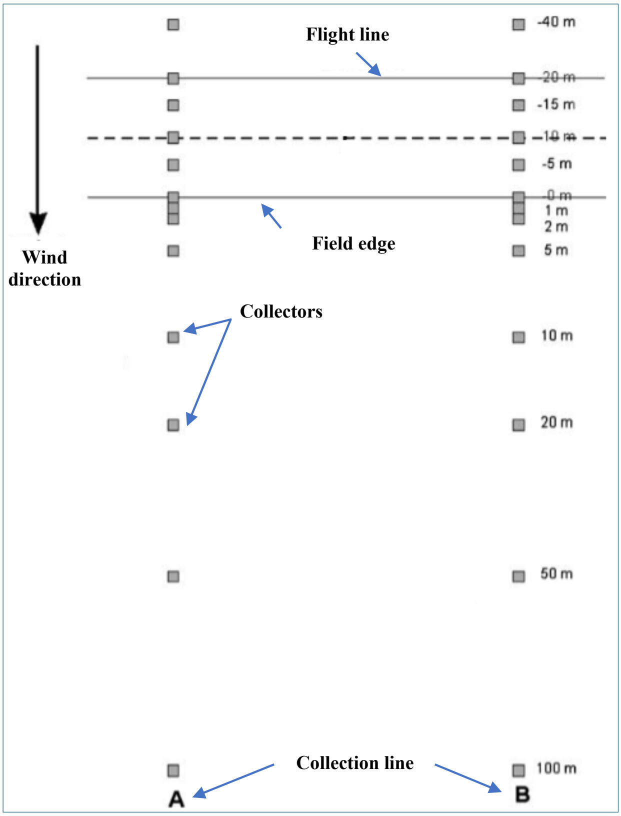


Fig. 6. Arrangement of collectors along collection lines A and B

Source: acc. to [43]

Data Collection and Analysis

White oil-sensitive papers measuring 52 mm × 76 mm were arranged in six lines at distances of 5, 10, 20, 30, 50, and 100 m from the edges of the treated fields; each line consisted of 20 collectors that were positioned 20 cm above the ground (Fig. 7), for a total of 120 collectors per site. The aircraft were prepared by positioning CP-11TT nozzles on their booms; the spraying was then carried out according to the defined flight lines. The operational and meteorological conditions of the investigated sites were recorded during the applications (Table 4).

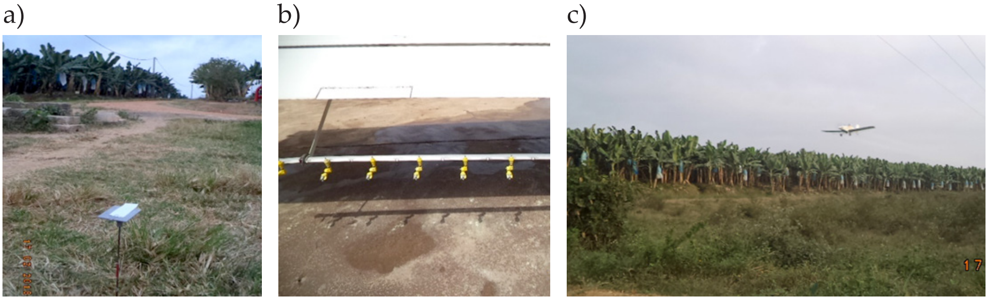


Fig. 7. Collection of pesticide-dispersion data in environment:
a) positioning oil-sensitive papers perpendicular to field;
b) positioning of CP-11TT nozzles on aircraft; c) application of fungicide in field

Table 4. Operational and meteorological conditions for spraying studied banana plantations

Parameter	BANACOMOE	SIAPA	BANACI	SAKJ	EGLIN
Aircraft model	Thrush 510/34	ULM	ULM	helicopter	helicopter
Nozzle type	CP-11TT	micronaires	micronaires	D6	D6
Number of nozzles	34	4	4	36	36
Ramp length [m]	10.26	8	6.7	7.2	7.2
Wing width [m]	14.57	11	9.2	8.2	8.2
Ramp/Wing ratio [%]	70.4	72	73	88	88
Flight speed [m·s^{-1}]	220	100	100	170	170
Porridge type	emulsion	pure oil	pure oil	emulsion	pure oil
Volume of mixture per hectare [L]	20	14	14	20	15
Slush color	yellowish	yellowish	yellowish	yellowish	whitish

Table 4. cont.

Parameter	BANACOMOE	SIAPA	BANACI	SAKJ	EGLIN
Fungicides (active matter)	fenpropimorph	fenpropimorph	fenpropimorph	mancozeb	thiophanate-methyl
Wind speed [m·s^{-1}]	2.8	0.0	0.4	0.7	0.8
Temperature [°C]	28.6	25.6	31.6	32.5	29.9
Relative humidity [%]	69.2	82.2	68.0	72.9	71.0
Wind direction	NE	NE	NE	SW/NE	NW/SE

After the pesticides were applied, the trays were immediately recovered, and the oil-sensitive papers were transferred to previously labeled sampling jars. The samples were analyzed in the laboratory by mass spectrometry coupled with liquid chromatography (LC-MS) in order to determine the quantity of the phytosanitary product that was deposited on each tray. This was an analysis that was done in different stages of the sample preparation, LC-MS analysis, and quantification according to Pitt [44]. The concentrations that were obtained at the end of the laboratory analysis were used to calculate the percentages of the deposition in relation to the total quantities that were sprayed.

2.4. Fitness Function

After a descriptive analysis of the data, field y_i and simulated y'_i values were compared with each other for each of the operational and meteorological conditions of the five Ivoirian banana plantations that were investigated. Field y_i and the simulated y'_i values thus constituted the two groups to be compared for each site. The normality of the data was checked by the Shapiro–Wilk test at a threshold of $p = 0.01$ [45]. For the normally distributed values, the homogeneity of the variances was evaluated by an F-test at a threshold of $p = 0.05$ [46]. The Kruskal–Wallis test [47] was used to assess the adequacy of the field y_i and the simulated y'_i values at each site whose data was not normally distributed at a significance level of $p = 0.05$.

Furthermore, the statistical parameters were calculated from widely applicable metrics that were also used by Chicco et al. [20] to evaluate the performance of the DRIMERA tool. For a population n of y_i data with their mean $\overline{y}$, these parameters were as follows:

- coefficient of determination (r^2):

$$r^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - y'_i)^2}{\sum_{i=1}^{n} (y_i - \overline{y})^2} \tag{14}$$

- root mean square error (RMSE):

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - y_i')^2} \tag{15}$$

- mean absolute error (MAE):

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - y_i'\right| \tag{16}$$

when r^2 was close to 1, the RMSE and MAE values were low, and the p-value was high; this indicated that there is no significant difference between the variances or medians between the real and simulated values and that the model was qualified as performing well [20]. In this case, the simulated data represented the phenomena that were actually observed at the sites.

3. Results and Discussion

3.1. Data Descriptive Analysis

After simulations with the DRIMERA software under the five sites' operational and meteorological conditions, the obtained results were in the form of the mass of the pesticide's active ingredient in the environment. By relating this data to the initial total mass of the active ingredient in the applied pesticide, it was converted into the pesticide-deposition rate as a function of distance; thus, we obtained a simulated deposition or drift rate data y_i'. Similarly, we obtained data on the deposition or drift rate in the y_i field by relating the concentrations that were obtained at the end of the laboratory analysis to the total quantity that was sprayed. The y_i and y_i' values for all of the sites at distance i are shown in Table 5.

Table 5. Simulated and field deposition data [%]

Site / Variable		Distance									
		10 m	20 m	30 m	40 m	50 m	60 m	70 m	80 m	90 m	100 m
BANACOMOE	y	20.00	26.00	24.00	13.00	6.00	7.00	0.00	0.00	0.00	0.00
	y'	25.14	27.90	27.07	20.64	10.93	3.41	0.53	0.03	0.00	0.00
SIAPA	y	30.00	10.00	10.00	18.00	10.00	5.00	0.00	0.00	0.00	0.00
	y'	24.97	24.59	22.56	17.48	10.15	3.99	0.93	0.14	0.01	0.00
BANACI	y	12.00	10.00	22.00	17.00	15.00	8.00	7.00	2.00	0.00	0.00
	y'	9.68	16.19	20.36	19.90	15.15	8.62	3.49	0.96	0.00	0.00

Table 5. cont.

Site / Variable		Distance									
		10 m	20 m	30 m	40 m	50 m	60 m	70 m	80 m	90 m	100 m
SAKJ	y	9.00	7.00	4.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	y'	10.84	9.43	4.90	1.29	0.17	0.01	0.00	0.00	0.00	0.00
EGLIN	y	20.00	9.00	13.00	22.00	24.00	0.00	0.00	0.00	0.00	0.00
	y'	30.21	32.56	32.71	30.57	25.36	17.18	8.72	3.12	0.70	0.02

The simulated y' (red) and field (blue) deposition-rate data is presented in histogram form (Fig. 8). At each site, the field (y) and simulated (y') deposition values evolved to be substantially identically as a function of distance – particularly, for the BANACOMOE, BANACI, and SAKJ banana plantations.

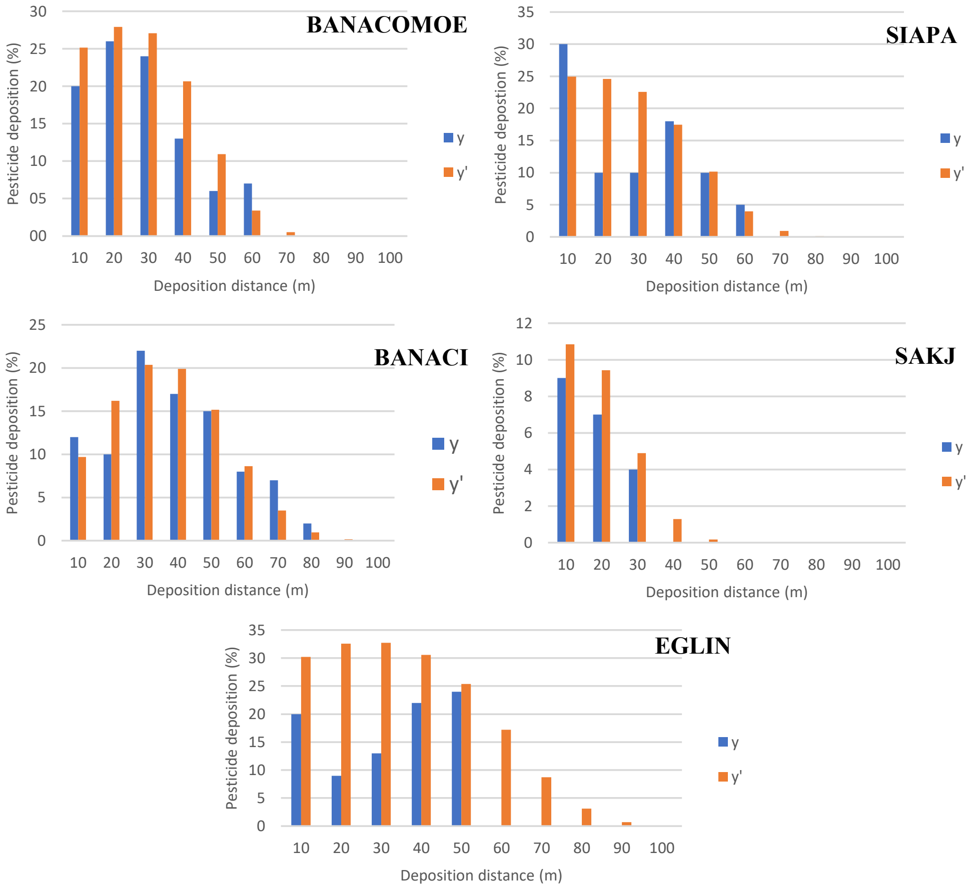


Fig. 8. Histogram of simulated y' (red) and field y (blue) pesticide depositions as function of distance

The field and simulated deposition data at the sites is described in Table 6. The *p*-values that were obtained by the Shapiro–Wilk test indicated that, at a threshold of 0.01, the observed and simulated values on the different sites were normally distributed (except at the SAKJ banana plantation). The medians of the observed and simulated data from the SAKJ site was, thus, evaluated by the Kruskal–Wallis test, while the variances of the observed and simulated data on the other sites was compared by the *F*-test.

Table 6. Descriptive statistics of field and simulated deposition data [%]

Site / Variable		Descriptive statistics					
		Mean	Std.	Min	Max	Range	*p*-value (Shapiro–Wilk test)
BANACOMOE	y	9.60	109.38	0.00	26.00	26.00	0.0427
	y'	11.56	151.46	0.00	27.90	27.90	0.0154
SIAPA	y	8.30	95.57	0.00	30.00	30.00	0.0327
	y'	10.48	118.19	0.00	24.97	24.97	0.0239
BANACI	y	9.30	54.90	0.00	30.00	30.00	0.6990
	y'	9.43	65.87	0.00	20.36	20.36	0.1665
SAKJ	y	2.00	11.78	0.00	9.00	9.00	0.0002
	y'	2.66	17.90	0.00	10.84	10.84	0.0006
EGLIN	y	8.80	103.96	0.00	24.00	24.00	0.0122
	y'	18.11	191.17	0.02	32.71	32.69	0.0482

3.2. Comparison of Field and Simulated Data

A statistical evaluation of the DRIMERA simulation data is presented in Table 7; it is clear that the quality of the results varied considerably from site to site. The obtained coefficient of determination r^2 values varied between 0.6331 and 0.9876 according to the different operational and meteorological simulation contexts. What is more, observations of the *p*-values showed that there was no significant differences among the variances on the one hand and the medians on the other (at a threshold of $p = 0.05$): the simulated data, therefore, represented the phenomena that was actually observed at all of the sites. However, the SAKJ site seemed to be the one where the DRIMERA model worked the best, with an r^2 level that was very close to 1 and with very low RMSE and MAE values. However, the results were not as good at the EGLIN site, with the lowest r^2 value and higher statistical errors. DRIMERA also made a prediction error of 9.31 (MAE) on the field-deposition data (expressed as a percentage).

Table 7. Coefficient of determination and statistical errors on data from sites [%]

Statistical errors	BANACOMOE	SIAPA	BANACI	SAKJ	EGLIN
r^2	0.9439	0.6762	0.8854	0.9876	0.6331
RMSE	3.6781	6.3112	2.6188	1.0858	12.2664
MAE	2.6830	3.4949	1.8370	0.6642	9.3143
p-value (F-test)	0.6356	0.5035	0.1467	–	0.5840
p-value (Kruskal–Wallis test)	–	–	–	0.4373	–

3.3. Discussion

DRIMERA's user interface features a quadrant for entering input data and another for viewing simulation results; in addition, a "Help" tab is available to facilitate the use of the application. This help is made available to users to assist and guide them in their tasks according to Bach et al. [48]. The aim was to make DRIMERA as easy to use as possible. Indeed, it is well known that the ease of use of an application is a real asset for its appropriation by users (as Jelassi and Hérault stated [49]). Consequently, the simplifications of complex atmospheric models (with a view to making them more accessible to users) was the key reason for the design of this application.

Furthermore, the results of the comparison between real and simulated data showed that DRIMERA was capable of accurately predicting pesticide drift under different weather conditions; the simulated data was, therefore, a good representation of the phenomena that were actually observed at all of the sites. Among these sites, the SAKJ site (which recorded the highest r^2 values and the lowest statistical errors [RMSE and MAE]) was the one where the DRIMERA model performed best. In fact, an r^2 close to 1 and a low number of statistical errors suggested a high-performance model. The model can therefore be used to assess the risk that is associated with aerial pesticide spraying in banana plantations. In contrast to the SAKJ site, the model performed less well at the EGLIN site, with a higher maximum error (9.31) and a lower r^2 value. The uncertainties that were reflected by these low r^2 values (also noted by Renaudo et al. r^2 [50]) could have been attributed to the stochastic nature of the atmospheric turbulence. Indeed, the instability in the airflow (which had significant effects on the mean flow velocity and the magnitude of the turbulent flows) made the drift models more complex (as Huang and Bou-Zeid stated [51]). This complexity is all the more pronounced in agricultural environments, where interactions between vegetation and atmosphere create heterogeneous microclimates. Although difficult to model, atmospheric turbulence remains one of the important parameters that influences pesticide drift (along with temperature and humidity); this was according to Kruger et al. [52]. Studies such as those by Katul et al. [53] have highlighted the difficulty of accurately modeling turbulence in near-surface areas due to the presence of coherent structures and the non-stationarity of the flows. In addition, the work of Finnigan [54] highlighted the importance of vegetation-atmosphere interactions in modifying wind profiles and turbulent flows; these directly affect the dispersion of pesticide particles.

The rotations of aircraft propellers can also have an impact on pesticide drift. Indeed, studies by Thomson et al. [55] showed an interaction between the vortex that is created by an aircraft propeller, the blast that is caused by this vortex, and the pesticide-deposition distance (at a significance threshold of $p = 0.10$). Drift tends to decrease when spraying with the propeller rotation and wind flow in the same direction [56]. Furthermore, little variability in pesticide deposition can be observed when the propeller vortex is in the same direction as the wind.

By combining an advanced Eulerian CFD (computational fluid dynamics) model with realistic droplet-distribution (Weibull distribution) and detailed meteorological data (wind rose), DRIMERA offers a more physically detailed modeling of pesticide drift. Indeed, it uses detailed Eulerian CFD modeling; this is unlike AgDRIFT® (which relies on semi-empirical models that are derived from field and wind-tunnel tests [57]) and XDrift (which is designed on a statistical approach that is derived from experimental data [58]). DRIMERA is, thus, capable of finely simulating airflows, providing a much more granular understanding of drift phenomena. Furthermore, the coupling of this advanced modeling with the Weibull distribution and the wind rose for droplet-size distribution allows for extremely detailed considerations of local meteorological conditions (which vary from site to site). DRIMERA thus allows for much higher spatial and temporal resolutions than empirical models such as AgDRIFT® or stochastic models such as XDrift (which cannot achieve the same precision). This approach thus makes it possible to better capture the complexities of air flows and droplet dispersions in varied environments.

4. Conclusion

The toxicity to human health and to the environment of pesticide motivated this study. The difficulty of obtaining field data for the organisms exposure assessment in the risk-assessment process can be resolved by modeling; so, a Euler coupled with Weibull's law and a wind rose-type model of atmospheric dispersion named DRIMERA was developed. Indeed, this decision-support tool brings the results of spatiotemporal dispersion predictions together, thus helping evaluate the exposures of target organisms to dangers and to characterize the associated risks.

From the comparison with the data that was observed in five Ivorian banana plantations in different operational and meteorological contexts, it emerged that the DRIMERA model simulated the phenomena that were observed on all sites quite well (at a threshold of 0.05). The values of coefficient of determination r^2 varied between 0.6331 and 0.9876, with the lower values being due to more-turbulent wind flows. The maximum error that was committed was 0.1227 on the simulated deposition values (translating to 1% of the real value). In addition, the variations in the scales of the deposition values only slightly influenced the errors. This model is, therefore, able to accurately predict pesticide drift under different weather conditions. The observed uncertainties are attributable to the stochastic nature of atmospheric turbulence and, to some extent, to the rotations of aircraft propellers.

For assessors who do not possess sufficient technical expertise to operate a state-of-the-art complex model system, DRIMERA represents real support. It helps facilitate a wider use and adaptation of atmospheric models.

Funding

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

CRediT Author Contribution

K. S.-P. K.: conceptualization, methodology, software, validation, formal analysis, data curation, writing – original draft preparation.

N. E. A.: investigation, resources, writing – review and editing, project administration.

Declaration of Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work that is reported in this paper.

Data Availability

Public Data: https://github.com/spkouadio/drimera_atmodel.

Use of Generative AI and AI-Assisted Technologies

No generative AI or AI-assisted technologies were employed in the preparation of this manuscript.

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