

Review of the Approach to Modelling Pesticides Dispersion in Environment for Determining the Concentrations to Which Organisms are Exposed as Part of Risk Assessment

Kouadio Kouassi Saint-Pierre* and Assidjo Nogbou Emmanuel
Laboratoire des Procédés Industrielles, de Synthèses, de l'Environnement et des Énergies Nouvelles, Institut National Houphouët Boigny, Yamoussoukro, Côte d'Ivoire

Abstract

There is an interest in the toxicity of pesticides in plant protection treatments for humans and the environment. As such, assessing toxicity risk is essential. Risk assessment is constrained due to the large amount of data to be measured, short collection times, insufficient data even when available, and the absence of bioaccumulation of the pollutant in the target organism. Modelling becomes an ally in overcoming these shortcomings. The assessor thus has at his disposal statistical, compartmental, Gaussian, Lagrangian, and Eulerian models to estimate the exposure of target organisms.

Keywords: Modeling, Pesticides, Aerial spraying, Risk assessment.

1. Introduction

To satisfy the growing demand for food, producing countries have relied mainly on increasing the harvested area. The increase in farm productivity, stimulated by the increase in demand, has been achieved through improved irrigation systems but above all through a marked increase in the use of fertilizers and especially pesticides [1]. Unfortunately, these pesticides have caused nearly 385 million cases of accidental non-fatal poisonings annually, including 11,000 deaths [2]. In addition, 8 to 17 out of every 100 people die from self-poisoning among the approximately 2 million cases annually. Several cases of cancer, childhood leukaemia and certain effects on the neurological, immunological and reproductive systems are linked to occupational or residential exposure to pesticides.

When used by aerial applications, pesticides can end up in the different physical and biological compartments of the environment because of the drift phenomenon [3]. It is therefore necessary to assess the risks associated with this agricultural technique. The data of pesticide concentrations in the different compartments of the environment are provided either from measurement or modelling. For the latter, the American Environmental Protection Agency US EPA and the WHO advocate the use of analytical approaches based on rigorous methods approved by the scientific community [4]. This is how publications on statistical analysis methods of environmental data, modelling of the dispersion and distribution of pollutants in the environment in this case, are emerging.

This article therefore proposes to summarize the conclusions on the main families of models used in the determination of concentrations of pesticides applied by air, as in the case of banana black leaf streak disease BLSA aerial treatment.

* Corresponding author.

E-mail address: kouadiostpierre@gmail.com

Manuscript History:

Received 25 February, 2023, Revised 18 September, 2023, Accepted 19 September, 2023, Published 31 October, 2023

Copyright © 2023 UNIMAS Publisher. This is an open access article under the CC BY-NC-SA 4.0 license.

<https://doi.org/10.33736/jaspe.5489.2023>

2. Risk assessment

Of controversial origin, the word "risk" has been strengthened over time by taking into account the psychological, sociological and economic dimensions [5] [6] to become the effect of an uncertain event (potential situation or scenario), resulting in exposure to danger or loss of something of value according to the definition given in Risk Management [7]. It can also prevent the achievement of an individual's or organization's objectives. Risk assessment, a useful step in risk analysis, is the following set of activities (Figure 1):

- Hazard identification is the identification of biological, chemical and/or physical agents that may cause adverse health and environmental effects ;
- Exposure assessment to establish the objective conditions of exposure of target organisms and therefore based on the determination of pesticide concentrations in the different compartments of the environment either from measurement or modelling;
- Danger characterization in which the goal is to determine reference levels via the analysis of the relations exposure-response associated with each potentially toxic compound. It allows one to determine the values without effect and the acceptable levels translated into Toxicological Reference Value (TRV).
- Risk characterization, which determines the level of risk by relating the exposure doses to the (eco)toxicological reference values of the contaminants using the RI risk index. It is thus the estimation, with possibly corresponding uncertainties, of the probability and the gravity of the harmful effects, known or potential, on health and the environment likely to occur.

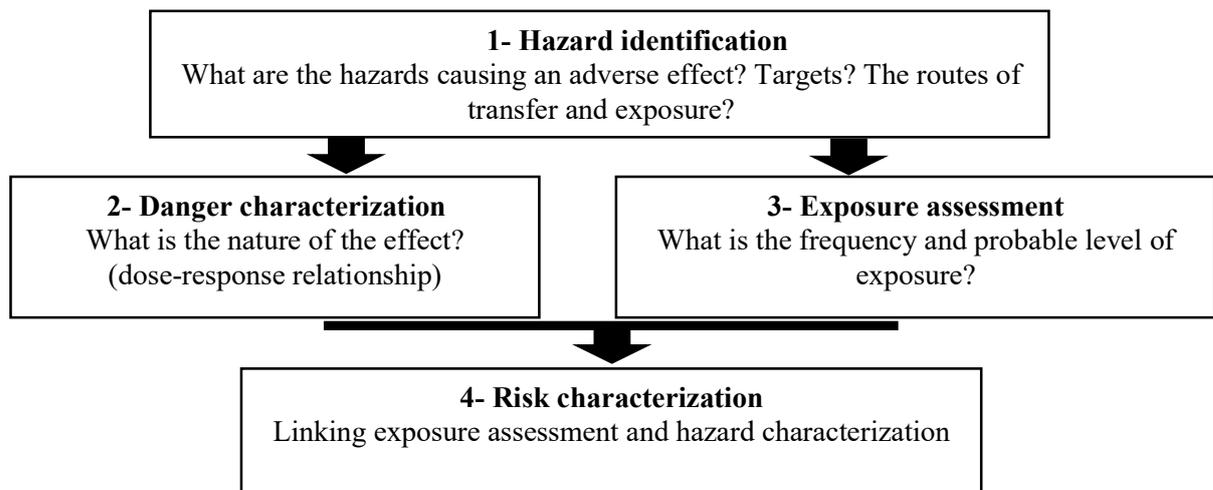


Figure 1. Risk assessment activities

According to Deram et Van Staevel [8], the two major concerns in risk assessment are the protection of the environment and the preservation of human health. It is based on risk prevention, risk forecasting and crisis management, and risk culture [9].

Risk assessment approaches are of two types: qualitative and quantitative [10] [11] [12]. According to Assidjo et al. [13], a qualitative assessment is a descriptive or categorical analysis of risk. It is therefore an "a priori" assessment of risk under limited conditions of data, time, and/or other resources. Quantitative assessment is more of an "a posteriori" assessment of risk. Based on the mathematical analysis of data, it is either a point estimate of simple values (average, extremes) or a

probability distribution of information characterizing the risk. The stochastic approach is preferred because it allows for a better appreciation, of the different levels of risk to which the population is exposed [13].

3. Constraints related to field data acquisition

The assessment of the exposure of target organisms, which consists of determining the (chemical) dose and/or dose rate of exposure based on knowledge of the nature and quantities of ingested and inhaled elements (food intake, respiratory rate, etc.), is not always easy by simply collecting data. Modelling thus becomes a substitute or complementary tool to the acquisition of field data [14]. In this case, it can be used to respond to various constraints encountered in the context of risk assessment [15] [14] [16] :

- A large amount of measurement data of pollutant concentrations in biotic and abiotic compartments. This represents technical difficulties and imposes significant financial and time costs. Modelling can then be used to predict exposure when it cannot be measured.
- The time required for sample collection, analysis and interpretation of results is sometimes incompatible with the need for a rapid diagnosis of the site's condition. Modelling thus allows preliminary information to be confirmed on the risk associated with the pollutants.
- insufficient data due to constraints in terms of human, financial and time requirements. The fragmented information (point measurements) can be completed due to modelling.
- absence of bioaccumulation of the pollutant by the target organism. Modelling allows exposure to be assessed when internal concentration measurements do not provide information on the dose.

4. Phenomenology of pesticide dispersion

Pesticides used during aerial treatments are introduced into the atmosphere by two main mechanisms: drift during application and volatilization, which can take place several days, weeks or even months after the treatment [3]. At the time of application, a part of the phytosanitary products does not reach the treated surfaces. Authors such as De Luca et al. [3] agree that this "loss of compounds" called drift is strongly influenced by the application methods as well as the climatic conditions (temperature, hygrometry, wind speed and direction). It varies in particular according to the physical properties of the spray applied, local conditions (topography of the land, type of soil), and the choice and adjustment of spraying equipment (height of booms, calibration of nozzles, etc.). In fact, the dispersion of pesticides in the atmosphere is related to the size of the sprayed droplets. Small drops can evaporate and become too light to settle.

Volatilization, defined as a physicochemical process by which a compound is transferred from the solid or liquid phase to the gas phase, can result from evaporation from the liquid phase, or sublimation from the solid phase. The Henry's constant evaluates the tendency of a product to volatilize.

In addition, the phenomena of degradation (decomposition, photolysis and photodecomposition), dry or wet deposition and transfer in the soil and hydrosystems give the possibility to pesticides to be distributed in the physical compartments (air, water, soil) and biological environment depending on the compound (solubility, vapour pressure, etc.) and the characteristics of the environment (air temperature, water, soil structure, humidity of the environment, etc.)

5. Dispersion models

The state-of-the-art on pesticide dispersion modelling is discussed by authors such as Unsworth et al. [17], Gil et Sinfort [18], Chahine [19], Brunet et al. [20]. In addition to the statistical models, we

distinguish among the deterministic models, the large families of compartmental models (box models), Gaussian, Lagrangian and Eulerian models. Some of these models incorporate parameterizations of phenomena such as volatilization and dry/wet deposition.

5.1. Statistical models

Statistical methods are used to build these models. They combine data obtained under controlled conditions with field results. Data from measurement campaigns conducted by the German *Biological Research Centre for Agriculture and Forestry* BBA resulted in a model for predicting terrestrial and aquatic drift and volatilization [21].

Based on these data, a model was developed by the European group FOCUS (*FORum for Co-ordination of Pesticide Fate Models and their Use*) by performing multi-regressions to calculate drift rates as a function of distance in different situations [22]. Percent drift is estimated by :

$$D_d = a(Z_d)^b \quad (1)$$

where a and b, are crop-related coefficients and Z_d drift distance.

A stochastic approach to modelling the particle trajectories of the projected jets was proposed by Smith et Miller [23]. An empirical model has also been proposed by Sarker et Parkin [24]. It predicts droplet drift based on the correlation between the most influential parameters in the drift process from tunnel measurements.

Teske et al. [25] model, which is the Level 1 drift assessment for terrestrial treatments in the AgDrift model developed by the US-EPA, estimates deposition rate as a function of distance x from the edge of the plot by :

$$D(x) = \frac{c}{(1+\frac{x}{a})^b} \quad (2)$$

where a, b and c are calibrated by experimental measurements.

5.2. Compartment or fugacity approach models

Developed during the 1980s [26], compartmental or multimedia-type models establish a flow between different environmental compartments (soil, plant, air, water) through partition coefficients ($K_{\text{leaf-atmosphere}}$, $K_{\text{soil-water}}$, ...) as a function of the ecosystem. These models are based on theoretical formulas describing the diffusion and advection processes such that the variation in time of pesticide concentrations is calculated by the mass balance equation (sum of advection, diffusion, source/sink).

$$\frac{\partial c}{\partial t} = -u_j \frac{\partial c}{\partial x_j} + \frac{\partial}{\partial x_j} \left(D \frac{\partial c}{\partial x_j} \right) + S + R \quad (3)$$

with c the pesticide concentration, D the molecular diffusion coefficient of the species, S the source term and R the production or destruction term by chemical reaction.

The advection term represents the mass flow of pesticide migrating from one compartment to another, the diffusion term represents the migration by turbulent and molecular transport due to concentration gradients. The source term is the entry into the pesticide compartment, the degradation term is mainly due to photolysis and microbiological transformations. Degradation generally follows a rate of order 1.

Note that for a given compartment i, the concentration of the pesticide is directly related to its fugacity parameter f_i (expressed in Pa) which explains the capacity of the pesticide to escape from the said compartment whose absorption capacity is Z_i (expressed in $\text{mol.m}^{-3}.\text{Pa}^{-1}$).

$$C_i = f_i Z_i \quad (4)$$

The partition coefficient between two compartments i and j can then be written :

$$K_{i,j} = \frac{z_i}{z_j} \quad (5)$$

The compartment models can be categorized into four (04) classes on the basis of, on the one hand, the spatial and temporal scales considered and, on the other hand, the processes taken into account [27].

5.2.1. Fugacity level I

These simplistic models consider the atmosphere and other environmental compartments as a closed, steady-state system [19]. Each of the major environmental compartments operates with a defined concentration of pesticides. No exchange with the atmosphere or degradation phenomena are considered. Therefore, Level I compartment models cannot allow for the estimation of pesticide residence time in the atmosphere and long-range transport.

5.2.2. Fugacity level II

The level II compartment models consider the atmosphere as an open system in a steady state. They take into account the dry and wet deposition phenomena in addition to the chemical reactivity of molecules. The source (input of pesticides) and destruction (output or degradation by chemical reaction of pesticides) terms are assumed to be balanced in the different compartments. In contrast to fugacity level I, these models estimate the residence time of pesticides in the atmosphere and the long-range transport of pesticides.

5.2.3. Fugacity level III

The conditions of the Level II compartment models are repeated here with compartments consisting of sub-compartments in equilibrium. However, the compartments themselves are not in equilibrium. Indeed, the different compartments are considered mixed. The assumption of mixing the compartments is only valid when the pesticides are distributed more rapidly in the sub-compartments than when the compartments are in equilibrium [28]. Concentrations are then determined once equilibrium is reached.

5.2.4. Fugacity level IV

Level IV compartmental models are of fairly high complexity. They take into account the variability within the same compartment. The source term is not necessarily constant. These models allow inter-seasonal comparison of pesticide concentrations in the atmosphere. Compartment models include the Behaviour Assessment Model BAM [29], PRZM [30] and the Pesticide Emission Model PEM [31] [32], all of which are 1D models with a perpendicular axis to the soil and which consider processes related to volatilization.

5.3. Gaussian models

The idealized plume from the source is the basis for Gaussian models (puff or plume). The advection-diffusion equation integrates into a Gaussian law with the assumption of spatiotemporal

invariance of the wind speed and turbulent diffusion. The exact solution of this equation in steady state ($(\partial c/\partial t)=0$) considering the conservation of the pesticide mass is therefore :

$$c(x, y, z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(\frac{-y^2}{\sigma_y^2}\right) \left[\exp\left(\frac{-(z-h_s)^2}{2\sigma_z^2}\right) + R \exp\left(\frac{-(z+h_s)^2}{2\sigma_z^2}\right) \right] \quad (6)$$

With $\sigma_y(x)$ and $\sigma_z(x)$, respectively the width and depth of the plume, h_s is the source height, Q is the source strength and R is the fraction of the plume reflected.

The first two terms describe the wind and plume shapes as Gaussian distributions with standard deviation $\sigma_y(x)$ and $\sigma_z(x)$, with maxima at $x = 0$ and $z = h_s$, respectively. The third term represents the plume reflection at the ground surface.

5.3.1. Gaussian Plume models

Plume models assume continuous point source emission. Pesticides are then emitted with a constant flow rate Q over time and the flow is at uniform velocity u . The size of the plume, which is generally conical in shape, is conditioned by the strength of the wind in width $\sigma_y(x)$, and the instability of the air along depth $\sigma_z(x)$. According to the wind speed and especially the different stability states of the atmosphere, a classification is made by Pasquill [33] [34]. Table 2 shows the different classes.

Table 1. Pasquill atmospheric stability class

Wind speed at 10 m (m/s)	Day (Incident solar radiation)			Night (Cloudiness)	
	High	Medium	Weak	Cloudy sky	Relatively clear sky
< 2	A	A-B	B	F	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
> 6	C	D	D	D	D

A: very unstable B: unstable C: slightly unstable D: neutral E: stable F: stable

This classification then allows Turner [35], Briggs [36], and Griffiths [37] to propose, for example, values for the dispersion parameters $\sigma_y(x)$ and $\sigma_z(x)$ (Table 2). The median line thus gives the maximum pesticide concentration.

Table 2. Plume dispersion parameters according to Pasquill-Turner and Briggs

Class	Pasquill-Turner		Briggs in rural areas		Briggs in urban areas	
	$\sigma_y(x)$	$\sigma_z(x)$	$\sigma_y(x)$	$\sigma_z(x)$	$\sigma_y(x)$	$\sigma_z(x)$
A	$0,215 x^{0,858}$	$0,01 + 0,467 x^{1,89}$	$0,25x$	$0,28x\sqrt{1 + 0,0001x}$	$0,30x\sqrt{1 + 0,001x}$	$0,40x\sqrt{1 + 0,0004x}$
B	$0,155 x^{0,889}$	$0,103 x^{1,11}$	$0,15x$	$0,20x\sqrt{1 + 0,0001x}$		
C	$0,105 x^{0,903}$	$0,066 x^{0,915}$	$\frac{0,10x}{\sqrt{1 + 0,0002x}}$	$0,14x\sqrt{1 + 0,0001x}$	$0,25x$	$0,28x\sqrt{1 + 0,0004x}$
D	$0,068 x^{0,908}$	$0,0315 x^{0,822}$	$\frac{0,07x}{\sqrt{1 + 0,0015x}}$	$0,10x\sqrt{1 + 0,0001x}$	$0,18x\sqrt{1 + 0,0003x}$	$0,20x\sqrt{1 + 0,0004x}$
for $x < 1$ km						
E	$0,050 x^{0,914}$	$0,0232 x^{0,745}$	$\frac{0,04x}{\sqrt{1 + 0,0003x}}$	$0,07x\sqrt{1 + 0,0001x}$	$0,10x\sqrt{1 + 0,0015x}$	$0,14x\sqrt{1 + 0,0004x}$
F	$0,034 x^{0,908}$	$0,0144 x^{0,727}$	$\frac{0,02x}{\sqrt{1 + 0,0003x}}$	$0,05x\sqrt{1 + 0,0001x}$		
for $x > 1$ km						
E	$0,050 x^{0,914}$	$-0,126 + 0,148 x^{0,150}$				
F	$0,034 x^{0,908}$	$-0,017 + 0,0312 x^{0,306}$				

* Corresponding author.
E-mail address: kouadiostpierre@gmail.com

Manuscript History:
Received 25 February, 2023, Revised 18 September, 2023, Accepted 19 September, 2023, Published 31 October, 2023
Copyright © 2023 UNIMAS Publisher. This is an open access article under the CC BY-NC-SA 4.0 license.
<https://doi.org/10.33736/jaspe.5489.2023>

e-ISSN: 2289-7771

5.3.2. Gaussian puff models

Unlike plume models, this type of Gaussian model considers the emission at a point source as discontinuous. The approach consists of discretizing the emission as a succession of instantaneous releases called "puffs". Each puff, whose centre of mass is advected by the velocity field assumed uniform at each instant but evolving in time, obeys equation (6). The concentration at a point is then calculated by the sum of the puffs at this point. This approach has the advantage of integrating scenarios as complex as the variation of the velocity field and the quantity of pesticides.

These stationary considerations imply a result valid only over a short period of time in idealized conditions of flat and homogeneous terrain, i.e. far from large shears and surface turbulence, but also far from the source due to the turbulence created by the spraying equipment. They provide good average estimates on scales of 0.5 to 10 km [38] [39].

Some models that take into account dry deposition, vertical variation in turbulent diffusivity, gas and liquid phases, and spatial wind heterogeneity have subsequently been developed. This is the case of the Industrial Source Complex Short Term ISCST model [40] and the Gaussian Diffusion and Sedimentation GDS [41] model.

5.4. Lagrangian models

The Lagrangian theory is built around the assumption of droplets independency considered spherical with a density greater than that of air and a diameter smaller than the Kolmogorov scale. The trajectory of the particle, calculated in these models, is initially dominated by its inertia and its speed of emission to be thereafter dictated by the wind speed and turbulence until its deposition on the vegetation or on the ground.

5.4.1. Wind speed

The average horizontal wind speed over the canopy is a function of height and canopy surface roughness [42] [43] according to equation (7) :

$$U(z) = \frac{u_*}{\kappa} \log \left(\frac{z-d_z}{d_r} \right) \quad (7)$$

with $U(z)$ wind speed at height z (m.s⁻¹), u_* friction velocity, $\kappa = 0.4$ von Karman constant, z height (m), d_z crop height (m) and d_r surface roughness (m).

This profile changes shape when inside the vegetation and becomes :

$$U(z) = \frac{U_c}{(1+\kappa(1-\frac{z}{z_c}))^2} \quad (8)$$

with $U(z)$ wind speed at height z_c (m.s⁻¹), z_c crop height (m) and $\kappa = 2$ constant depending on the canopy structure.

5.4.2. Initial velocity of droplets

* Corresponding author.

E-mail address: kouadiostpierre@gmail.com

Manuscript History:

Received 25 February, 2023, Revised 18 September, 2023, Accepted 19 September, 2023, Published 31 October, 2023

Copyright © 2023 UNIMAS Publisher. This is an open access article under the CC BY-NC-SA 4.0 license.

<https://doi.org/10.33736/jaspe.5489.2023>

e-ISSN: 2289-7771

The Bernoulli equation is used to calculate the velocity V_0 (9) of droplet emission on the basis of simplifying assumptions such as the knowledge of the position of the source and the distribution of initial velocities, the sphericity and the density constant of the particles, the immediate formation of the droplets at the nozzle exit.

$$V_0 = \sqrt{\frac{2 v_e P}{\rho_l}} \quad (9)$$

With v_e efficiency of the atomization process, P (m) pressure at the nozzle outlet and ρ_l ($\text{kg}\cdot\text{m}^{-3}$) droplet density.

Some authors [44] [25] have optimized this velocity by taking into account the turbulence caused by the pressure created in the vicinity of the nozzle with experimental data.

5.4.3. Equations of motion

The application of Newton's second law to the droplet with gravity, buoyancy and drag as forces in action allows us to write the differential equation of motion of the droplet in an air stream as follows :

$$\frac{dV}{dt} = g \frac{\rho_l - \rho_a}{\rho_l} - \frac{\rho_a \pi d^2 C_d V^2}{8(\rho_l \frac{\pi d^3}{6})} \quad (10)$$

with ρ_a air density, g gravity intensity, d droplet diameter, C_d drag coefficient.

5.4.3.1. Expression of the equilibrium velocity

The sedimentation velocity of the droplet obtained at equilibrium ($(dv/dt)=0$), in conditions close to the ground where the wind motion is horizontal, is written :

$$V_s = \sqrt{\frac{4}{3} \frac{g}{C_d} \frac{\rho_l - \rho_a}{\rho_a} d} \quad (11)$$

The velocity of the droplet then depends only on its size.

The drag coefficient C_d is related to the Reynold's number Re by the empirical relation on spheres recommended by [45] :

$$\begin{cases} C_d = \frac{24}{Re} (1 + 0.14Re^{0.70}) \text{ for } Re \leq 1000 \\ C_d = 0.447 \text{ for } Re > 1000 \end{cases} \quad (12)$$

Several other expressions are proposed by authors such as Holterman et al. [44], Reichard et al. [46] for values of $Re \leq 10^4$.

5.4.3.2. Effect of turbulence on velocity

When we move away from the ground, the knowledge of the instantaneous wind speed or turbulence becomes both essential and problematic. Indeed, it represents the difficulty in solving the equations of motion. It is, on the one hand, the general turbulence of the atmospheric boundary layer and on the other hand, the turbulence generated by the moving spray and by the air entrained inside the spray [47].

Xu et al [48] report on the methods of calculating the trajectory of droplets with consideration of turbulence. The two main ones are the random walk models and the RANS (Reynolds Averaged Navier-Stokes) models.

- **Random walk approach**

The trajectory of the droplet is obtained by a Markov process. Indeed, a relation between the velocities of the present t and previous $t - \Delta t$ instants, weighted by a random term due to the fluctuations of the air speed allows to take into account the turbulence.

Holterman et al. [44] propose the IDEFICS model :

$$\vec{V}_{i+1} = \vec{V}_i \alpha_i + \vec{V}_{s,i} (1 - \alpha_i) \text{ avec } \vec{V}_{s,i} = \tau_i \vec{g} + \vec{u}_i \text{ et } \tau_i = \frac{4\rho_l d_i}{3\rho_a V_i C_d} \quad (13)$$

where at time i , $V_{s,i}$ is the sedimentation velocity, u_i is the wind speed, and τ_i is the droplet relaxation time.

The wind speed u_i is the combination of the average air speed and a local random speed calculated from atmospheric stability.

- **Reynolds Averaged Navier-Stokes (RANS) model**

The RANS method, much used in fluid mechanics for turbulent flows, is an approach to solutions of the Navier-Stokes equations by the Reynolds average which is the statistical average of the arithmetic mean of the flow [47] [49]. We then obtain the so-called Reynolds equation :

$$\rho \left(\frac{\partial}{\partial t} + \bar{u}_j \frac{\partial}{\partial x_j} \right) \bar{u}_i = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \bar{u}_i}{\partial x_j} - \overline{\rho u'_i u'_j} \right) \quad (14)$$

with ρ density and μ dynamic viscosity of the droplet.

The Reynolds tensor $\overline{\rho u'_i u'_j}$ comes from the nonlinearity of the Navier-Stokes equations and reflects the mean effect of turbulence through interactions between mean and fluctuating motion. A solution lies in the Boussinesq closure assumption which models the Reynolds tensors using a turbulent viscosity μ_t whose expression in the popular k - ε model is :

$$\mu_t = C_\mu \frac{k^2}{\varepsilon} \quad (15)$$

With k , turbulent kinetic energy and ε , viscous dissipation rate.

The evaporation phenomenon is considered in some works [50] [51] [52] [53] [54]. All of them are based on the Ranz et Marhsall [55] [56] model used in the CFD computational code Fluent®.

The Lagrangian type model thus allows the simulation of the dispersion on heterogeneous grounds and with the physicochemical transformations of the droplets. We can mention the model proposed by Walklate [57], Driftsim [46], IDEFICS [44] and the level 2 of the AgDrift model [25].

5.5. Eulerian models

In Eulerian models, the approach consists in a numerical solution of the advection-diffusion equation discretized in space and time. The knowledge of the initial conditions in time and the boundary conditions of the spatial domain are then essential.

5.5.1. Pollutant concentration

After meshing air into multidimensional cells, the concentration of the pollutant is determined in each cell based on the inflow and outflow from Navier-Stokes equations. The solution is then

approximated by the Reynolds decomposition and the RANS method as with the Lagrangian models. Equation (16) gives the expression for the average concentration:

$$\frac{\partial \bar{c}}{\partial t} = -\bar{u}_j \frac{\partial \bar{c}}{\partial x_j} + \frac{\partial}{\partial x_j} \left(D \frac{\partial \bar{c}}{\partial x_j} - \overline{u'_j c'} \right) + \bar{S} + \bar{R} \quad (16)$$

Pesticides global movement is thus followed with respect to a fixed reference frame. Moreover, this assumes the knowledge of the velocity and turbulence at any point of the chosen mesh.

5.5.2. Modeling of the turbulent flow

The most common approach to calculate the turbulence field is the modelling by a first-order closure of Boussinesq. It consists of expressing the turbulent flows as a function of the gradient of the mean quantities :

$$\overline{u'_j c'} = k \nabla \bar{c} \quad (17)$$

With k obtained in equation (15)

Eulerian-type models can thus obtain pesticide concentrations a few days after spraying even at the regional level. Examples are EUROS [58], MATCH [59], ASIMD [60].

6. Applications of drift modelling

Drift modelling has allowed a tremendous advance in improving operational parameters and optimizing spray conditions [61] [3] but also in risk assessment especially [62] [63]. Indeed, the collective and growing awareness of the potential risks of exposure of organisms to pesticides through drift has prompted the development of mitigation measures. For example, a modelling study conducted by Ganzelmeier et al [64] led to a tool that allowed its authors to propose a safety zone (untreated area around the agricultural plot) depending on the type of nozzles and pesticides used. This model is based on drift measurement campaigns during phytosanitary treatments of different crops, namely field crops, viticulture, arboriculture and hops. In addition, based on data from the BBA (now BVL for « *Bundesamt für Verbraucherschutz und Lebensmittelsicherheit* ») model [64] [65], the European working group FOCUS assesses the risk of pollution of surface waters. In a report on aquatic risk assessment [66] [67], FOCUS recommends mitigation measures on the use of safety zones, the application of drift reduction techniques and the use of windbreaks

In addition, the US Environmental Protection Agency (US EPA) has developed the AgDrift software, of which its level 2 aerial crop protection module estimates drop trajectories for aerial spraying [68]. Used in the United States and Canada, it is sufficiently documented and remains one of the tools recommended by international bodies to serve as a basis for risk assessments according to Piché [69].

7. Conclusion

The agricultural technique of aerial spraying gives pesticides the possibility, especially through the phenomenon of drift, to end up in the air, the soil, surface water and groundwater. It is necessary to evaluate the potential risks. In a risk assessment approach, the exposure assessment is based on data obtained by measurement campaigns or by modelling. The constraints linked to the large amount of data to be measured and the short time required for the collection, the lack of data even when available, and the absence of bioaccumulation of the pollutant in the target organism make modelling a complementary tool or a substitute for data collection. The assessor has at his disposal a wide range of models from the statistical, compartmental, Gaussian, Lagrangian and Eulerian families.

Conflict of interest

The authors have no competing interests to declare that are relevant to the content of this article.

References

- [1] OCDE/FAO. (2020). *Perspectives agricoles de l'OCDE et de la FAO 2020-2029*, Éditions OCDE, Paris/FAO, Rome. <https://doi.org/10.1787/ccc6f09c-fr>
- [2] UNEP. (2020). Environmental and health impacts of pesticides and fertilizers and ways of minimizing them - Envisioning a chemical-safe world.
- [3] De Luca, M., Vallet, A., Borghi, R. (2007). Contribution à la modélisation de la pulvérisation d'un liquide phytosanitaire en vue de réduire les pollutions. Journée Interdisciplinaires sur la Qualité de l'Air, Jan 2007, Villeneuve d'Ascq, France. 10 p
- [4] Carrier, G., & Bard, D. (2003). Analyse du risque toxicologique. *Environnement et santé publique – Fondements et pratique*. pp203-226. Edisem / Tec & Doc, Acton Vale / Paris
- [5] Taylor-Gooby, P., & Zinn, J. O. (2006). *Risk in Social Science*, New York, Oxford University Press.
- [6] Renn, O. (2008). *Risk Governance: Coping with Uncertainty in a Complex World* (1st ed.). Routledge.London. <https://doi.org/10.4324/9781849772440>
- [7] ISO. (2009). "Management du risque – Vocabulaire", ISO Guide 73, Organisation internationale de la normalisation, Genève.
- [8] Deram, A., & Van Staevel, E. (2006). Evaluation et acceptabilité des risques environnementaux. Synthèse de l'étude. Etude record n°04-0810//0811/1A. Juillet 2006
- [9] Gendreau, N., & Oberlin, G. (1998). Modélisation de synthèse des crues : modèles hydrologiques en débit-durée-fréquence et modèles hydrauliques. *Revue Ingénieries – eau, agriculture, territoires – n° spécial 1998 « risque naturels » du CEMAGREF : Risques naturels : avalanches, crues, inondations, laves, torrentielles, incendies de forêt*, 79-85
- [10] Jaykus, L. A. (1996). The application of quantitative risk assessment to microbial food safety risks. *Critical reviews in microbiology*, 22(4), 279-293. <https://doi.org/10.3109/10408419609105483>
- [11] Chen, Y., Jackson, K. M., Chea, F. P., & Schaffner, D. W. (2001). Quantification and variability analysis of bacterial cross-contamination rates in common food service tasks. *Journal of food protection*, 64(1), 72-80. <https://doi.org/10.4315/0362-028X-64.1.72>
- [12] Ferrier, S., (2002). Extended statistical approaches to modelling spatial pattern in biodiversity: the north-east New South Wales experience. II. Community-level modelling. *Biodiversity & Conservatio.*, 11: 2309-2338. <https://doi.org/10.1023/A:1021374009951>
- [13] Assidjo, E., Sadat, A., Akmel, C., Akaki, D., Elleingand, E., & Yao, B. (2013). L'analyse des risques: outils innovant d'amélioration de la sécurité sanitaire des aliments''. *Revue Africaine de sante et production animales, Dakar*.
- [14] BRGM, INERIS, ADEME, (2006). « Mesures » et « Modèles » : enjeux, avantages et inconvénients en contexte de gestion de sites pollués. BRGM EPI/ENV n°167/2006, INERIS DRC-75999-DESP 39/06, p.4.
- [15] European Commission EC, (2003). *Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market*. Version 2. European Chemical Bureau, 311.
- [16] van den Brink, N. W., Baveco, H., Bervoets, L., Perry, H., Vermeulen, F., de Winter, W., & van der Pol, J. (2007). Breaking ecotoxicological restraints in spatial planning (BERISP)-Manual for the BERISP-DSS. *Alterra, Wageningen, The Netherlands*, 72.

- [17] Unsworth, J. B., Wauchope, R. D., Klein, A. W., Dorn, E., Zeeh, B., Yeh, S. M., Akerblom, M., Racke, K.D. & Rubin, B. (1999). Significance of the long range transport of pesticides in the atmosphere. *Pure and applied chemistry*, 71(7), 1359-1383. <https://doi.org/10.1351/pac199971071359>
- [18] Gil, Y., & Sinfort, C. (2005). Emission of pesticides to the air during sprayer application: A bibliographic review. *Atmospheric Environment*, 39(28), 5183-5193. <https://doi.org/10.1016/j.atmosenv.2005.05.019>
- [19] Chahine, A., (2011). Modélisation de la dispersion aérienne de pesticides des échelles locales aux échelles régionales, influence des aménagements et quantification des niveaux d'exposition. Thèse de Doctorat. Centre International d'Etude Supérieures en Sciences Agronomiques, Montpellier SupAgro.
- [20] Brunet, Y., Dupont S., Chahine A. & Sinfort C. (2013). MODAPEX : Modélisation de la dispersion aérienne des pesticides et des niveaux d'exposition à l'échelle du paysage, programme « évaluation et réduction des risques liés à l'utilisation des pesticides », rapport scientifique.
- [21] BBA. (2002). *Programm zur abschätzung der abdrift und verflüchtigungsbedingten deposition von psm wirkstoffen im nichtzielbereich nach freilandanwendungen*. Tech. rep., BBA Germany
- [22] Boesten, J., Businelli, M., Delmas, A., Gottesbüren, B., Hanze, K., Jarvis, T., Jones, R., Klein, M., van der Linden, T., Rekolainen, S., Ressler, H., Roquero, C., Maier, W-M., Styczen, M., Thorsen, M., Travis, K. & Vanclooster, M. (2000). FOCUS groundwater scenarios in the EU review of active substances. *Report of the FOCUS groundwater scenarios workgroup, EC document reference sanc0/321/2000 rev, 2*, 202.
- [23] Smith, R. W., & Miller, P. C. H. (1994). Drift predictions in the near nozzle region of a flat fan spray. *Journal of Agricultural Engineering Research*, 59(2), 111-120. <https://doi.org/10.1006/jaer.1994.1068>
- [24] Sarker, K. U., & Parkin, C. S. (1995). Prediction of spray drift from flat-fan hydraulic nozzles using dimensional analysis. In *Brighton Crop Protection Conference Weeds* (Vol. 2, pp. 529-536). Brit Crop Protection Council.
- [25] Teske, M.E., Valcore, D.L. & Hewitt, A. (2001). An analytical ground sprayer model. ASAE Annual International Meeting Sponsored by ASAE 01-1051. <https://doi.org/10.13031/2013.7313>
- [26] Atmo Auvergne-Rhône-Alpes. (2017). *Pesticides dans l'air – Bibliographie sur la modélisation*. Juillet 2017
- [27] Smaranda, C., & Gavrilesco, M. (2008). Migration and fate of persistent organic pollutants in the atmosphere-a modelling approach. *Environmental Engineering & Management Journal (EEMJ)*, 7(6). ISSN 1582 - 9596
- [28] Devillers, J., Bintein, S., & Karcher, W. (1995). CHEMFRANCE: a regional level III fugacity model applied to France. *Chemosphere*, 30(3), 457-476. [https://doi.org/10.1016/0045-6535\(94\)00425-T](https://doi.org/10.1016/0045-6535(94)00425-T)
- [29] Jury, W. A., Spencer, W. F., & Farmer, W. (1983). *Behavior assessment model for trace organics in soil: I. Model description*, 12(4), 558-564). American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America. <https://doi.org/10.2134/jeq1983.00472425001200040025x>
- [30] Suárez, L. A. (2005). PRZM-3, a model for predicting pesticide and nitrogen fate in the crop root and unsaturated soil zones: users manual for release 3.12. 2. *US Environmental Protection Agency (EPA), Washington, DC*.
- [31] Scholtz, M. T., Voldner, E., McMillan, A. C., & Van Heyst, B. J. (2002). A pesticide emission model (PEM) Part I: model development. *Atmospheric Environment*, 36(32), 5005-5013. [https://doi.org/10.1016/S1352-2310\(02\)00570-8](https://doi.org/10.1016/S1352-2310(02)00570-8)
- [32] Scholtz, M. T., Voldner, E., Van Heyst, B. J., McMillan, A. C., & Pattey, E. (2002). A pesticide emission model (PEM) Part II: model evaluation. *Atmospheric Environment*, 36(32), 5015-5024. [https://doi.org/10.1016/S1352-2310\(02\)00571-X](https://doi.org/10.1016/S1352-2310(02)00571-X)
- [33] Pasquill, F. (1974) *Atmospheric diffusion: the dispersion of windborne material from industrial and other sources*. E. Horwood.
- [34] Pasquill, F. (1974). *Atmospheric Diffusion, 2nd edition*. London: Ellis Horwood Ed.
- [35] Turner, D.B. (1994). *Workbook of Atmospheric Dispersion Estimates: An Introduction to Dispersion Modeling, Second Edition*. CRC Press. <https://doi.org/10.1201/9780138733704>

- [36] Briggs, G. A. (1973). *Diffusion estimation for small emissions. Preliminary report* (No. TID-28289). National Oceanic and Atmospheric Administration, Oak Ridge, Tenn.(USA). Atmospheric Turbulence and Diffusion Laboratory.
- [37] Griffiths, R. F. (1994). Errors in the use of the Briggs parameterization for atmospheric dispersion coefficients. *Atmospheric Environment*, 28(17), 2861-2865. [https://doi.org/10.1016/1352-2310\(94\)90086-8](https://doi.org/10.1016/1352-2310(94)90086-8)
- [38] Thistle, H. (2000). *The role of stability in fine pesticide droplet dispersion in the atmosphere: a review of physical concepts*. Transactions of the ASAE 46, 1409-1413. <https://doi.org/10.13031/2013.3038>
- [39] Teske, M. E., Bird, S. L., Esterly, D. M., Curbishley, T. B., Ray, S. L., & Perry, S. G. (2002). AgDrift®: A model for estimating near-field spray drift from aerial applications. *Environmental Toxicology and Chemistry: An International Journal*, 21(3), 659-671. <https://doi.org/10.1002/etc.5620210327>
- [40] USEPA. (1995). *Users guide for the industrial source complex (ISC3) dispersion models. Vol.I- Users instructions*. EPA-454/B-95-003a, Sept. 1995. USEPA Office of Air Quality Planning and Standards Emissions, Monitoring, and Analysis Division, Research Triangle Park, NC.
- [41] Craig, I. P. (2004). The GDS model—a rapid computational technique for the calculation of aircraft spray drift buffer distances. *Computers and Electronics in Agriculture*, 43(3), 235-250. <https://doi.org/10.1016/j.compag.2004.02.001>
- [42] Thom, A. S. (1975). Momentum, mass and heat exchange of plant communities. *Vegetation and the Atmosphere*, 4, 57-109.
- [43] Hartley, G. S., & Graham-Bryce, I. J. (1980). *Physical principles of pesticide behaviour*, 1(2). Academic Press Inc.(London) Ltd..
- [44] Holterman, H. J., Van de Zande, J. C., Porskamp, H. A. J., & Michielsen, J. M. G. P. (1998). IDEFICS: a physical model of spray drift from boom sprayers in agriculture. *ILASS-Europe, Manchester*.
- [45] Perry, R., Green, D. & Maloney, J. (1984). *Perry's Chemical Engineers' Hand-book*.
- [46] Reichard, D. L., Zhu, H., Fox, R. D., & Brazee, R. D. (1992). Wind tunnel evaluation of a computer program to model spray drift. *Transactions of the ASAE*, 35(3), 755-758. <https://doi.org/10.13031/2013.28658>
- [47] Bahrouni, H. (2010). *Caractérisation de l'efficacité technique des systèmes de pulvérisation et des pertes de pesticides appliqués aux cultures basses dans les régions méditerranéennes : cas de la Tunisie*. Doctorat Agronomie, Spécialité : Génie des procédés, Montpellier SupAgro et INAT
- [48] Xu, Z. G., Walklate, P. J., Rigby, S. G., & Richardson, G. M. (1998). Stochastic modelling of turbulent spray dispersion in the near-field of orchard sprayers. *Journal of Wind Engineering and Industrial Aerodynamics*, 74, 295-304. [https://doi.org/10.1016/S0167-6105\(98\)00026-9](https://doi.org/10.1016/S0167-6105(98)00026-9)
- [49] Belhadef, A. (2010). *Contribution à la modélisation Eulérienne de l'atomisation pour la pulvérisation agricole*. Thèse de doctorat, Mécanique des fluides. Université de Provence - Aix-Marseille I, 2010.
- [50] Goering, C. E., Bode, L. E., & Gebhardt, M. R. (1972). Mathematical modeling of spray droplet deceleration and evaporation. *Transactions of the ASAE*, 15(2), 220-0225. <https://doi.org/10.13031/2013.37871>
- [51] Williamson, R. E., & Threadgill, E. D. (1974). A simulation for the dynamics of evaporating spray droplets in agricultural spraying. *Transactions of the ASAE*, 17(2), 254-261. <https://doi.org/10.13031/2013.36835>
- [52] Holterman, H. J., Van De Zande, J. C., Porskamp, H. A. J., & Huijsmans, J. F. M. (1997). Modelling spray drift from boom sprayers. *Computers and electronics in agriculture*, 19(1), 1-22. [https://doi.org/10.1016/S0168-1699\(97\)00018-5](https://doi.org/10.1016/S0168-1699(97)00018-5)
- [53] Brown, R. B., & Sidahmed, M. M. (2001). Simulation of Spray Dispersal and Deposition from a Forestry Airblast Sprayer---Part II: Droplet Trajectory Model. *Transactions of the ASAE*, 44(1), 11-17. <https://doi.org/10.13031/2013.2298>
- [54] Asman, W., Jørgensen, A., Jensen, P. (2003). *Dry deposition and spray drift of pesticides to nearby water bodies*. Tech. rep., Danish Protection Environmental Agency
- [55] Ranz, W. E., & Marshall, W. R. (1952a). Evaporation from drops. *Chemical Engineering Progress*, 48, 41-146.

- [56] Ranz, W.E. & Marhsall Jr., W.R. (1952b). Evaporation from drops, part II. *Chemical Engineering Progress* 48 (4), 173-180.
- [57] Walklate, P. J. (1992). A simulation study of pesticide drift from an air-assisted orchard sprayer. *Journal of Agricultural Engineering Research*, 51, 263-283. [https://doi.org/10.1016/0021-8634\(92\)80042-Q](https://doi.org/10.1016/0021-8634(92)80042-Q)
- [58] Van Pul, W.A.J., Jacobs, C.M.J., Van Jaarsveld, J.A. (1996). Air Pollution Modelling and its Application. *Ed. Gryning and Schiermeyer* : XI. Plenum Press, New York, 203–212.
- [59] Persson, C., & Ullerstig, A. (1996). *Model calculations of dispersion of lindane over Europe*. SMHI 68.
- [60] Pekar, M., Van Pul, W. A. J., & Borrell, P. M. (1998). Modelling of lindane and PCBs transport in the European region. In *Proceedings EUROTRAC symposium* (Vol. 98) Garmisch-Partenkirchen. In press
- [61] Sinfort, C., & Vallet A. (2003). Modeling the Dispersion of Pesticides during Applications: Ingénieries-EAT, Special Issue. *Technologies for sustainable agro* ; 85-94.
- [62] Sinfort, C., & Bonicelli, B. (2011). *Mesure et modélisation de la dispersion des pesticides dans l'air au voisinage des parcelles agricoles*. Anses, Bulletin de veille scientifique n°14, Santé / Environnement / Travail, Juin 2011. 18-21
- [63] Hilz, E., & Vermeer, A. W. (2013). Spray drift review: The extent to which a formulation can contribute to spray drift reduction. *Crop Protection*, 44, 75-83. <https://doi.org/10.1016/j.cropro.2012.10.020>
- [64] Ganzelmeier, H., Rautmann, D., Spangenberg, R., Streloke, M. (1995). *Studies on spray drift of plant protection products*, Mitteilungen aus der Biologischen Bundesanstalt für Landund Forstwirtschaft, Berlin Dahlem.
- [65] Rautmann, D., Streloke, M., & Winkler, R. (1999, September). New basic drift values in the authorization procedure for plant protection products. In *Workshop on risk management and risk mitigation measures in the context of authorization of plant protection products*. 133-141. ISSN 0067-5849
- [66] FOCUS. (2007a). *Landscape and mitigation factors*. In: *Aquatic Risk Assessment. Extended Summary and Recommendations*, vol. 1, Report of the FOCUS Working Groupon Landscape and Mitigation Factors in Ecological Risk Assessment. EC Document Reference SANCO/10422/2005 V.2.0, 1-169.
- [67] FOCUS. (2007b). *Landscape and mitigation factors*. In: *Aquatic Risk Assessment. Detailed Technical Reviews*, vol. 2, Report of the FOCUS Working Group on Landscape and Mitigation Factors in Ecological Risk Assessment. EC Document Reference SANCO/10422/2005 V.2.0, 1-436.
- [68] Teske, M. E., & Thistle, H. W. (1999). Poultry a simulation of release height and wind speed effects for drift minimization. *Transactions of the ASAE*, 42(3), 583-591. [doi: 10.13031/2013.13218](https://doi.org/10.13031/2013.13218)
- [69] Piché, M. (2014). *Acquisition de connaissances sur l'application de pesticides par voie aérienne – hélicoptère*. Programme Prime-Vert, Sous-volet 3.1 – Approche régionale. 46p