Computational decision-making support tool for the optimized application of phytopharmaceuticals

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Abstract— **Nowadays, agriculture deals with intensive production, plagues, pests and inefficient use of natural and energy resources, also due to global temperature increase and climate change. This work seeks to answer the need to create new decision support tools for the application of phytopharmaceuticals. Mathematical objective functions capable of answering two problems were gathered. The first simulates the route and life cycle of a phytopharmaceutical. The second objective function provides the ideal quantities of phytopharmaceutical to be applied, based on climatic conditions, temperature, size of the tree canopy and dimensions of the agricultural fields.**

Keywords – Computational decision-making tool, phytopharmaceuticals, dispersion, glyphosate, optimization, python.

I. INTRODUCTION

Agriculture has suffered a huge pressure to be able to respond to the most varied challenges. These challenges include intensive exploitation in agricultural production, increasing pesticide use and inefficient use of natural and energy resources [1]. One of these problems are the increasing number of plagues and pests, resistant to former chemical compounds, global temperature increase and climate change. To deal with this problem, but trying to reduce environmental impact while improving cultures sustainability, pesticides are continuously developed. These chemicals are essentially applied in cultures for the purpose of controlling this type of threats [1], [2]. One of the most successful pesticides globally in the elimination of plagues is glyphosate. Glyphosate (*N-(phosphonomethyl) glycine*) is a non-selective pesticide, wide spectrum, originally introduced in 1974, under the trade name of Roundup®, produced by a company named Monsanto. The intake mechanism of glyphosate is by absorption, either by the leaf intake in plants, the stem intake or root intake. The glyphosate that turns out to be dispersed in the surrounding environment, can then follow different paths: be absorption by the ground, degraded by microorganisms or absorbed by other plants [3]. There are also studies that suggest that the presence of glyphosate in aquatic ecosystems occurs by a transport phenomenon, be it by adsorption/desorption phenomena. It can also make the reverse path, reaching agricultural crops, ending up to affect the quality of the edible products produced [4]. This is amongst the herbicides with greater worldwide dissemination, with an annual consumption that ascends to 700,500 million kg [3], [4]. As all pesticides, its use entails problems for the environment [5]. Different studies indicate that the use of pesticides and fertilizers is amongst the main causes to the reduction of flora of the natural habitats adjacent to the agricultural fields [6].

Another problem is the dispersion of pesticides for non-target areas. This dispersion may vary from 1 to 25% of the applied pesticide, where factors such as disperser equipment, atmospheric conditions, application distance from the application point to the limits of the fields and the dimension of vegetation are responsible for the occurrence of a phenomena of sub application or excessive application of phytopharmaceuticals [6].

II. STATE OF THE ART

There have been some research studies that cover the use of decision-making tools for the optimization of agricultural activities using artificial intelligence techniques and other meta-heuristic methods. Nasri et al. [7] proposed the deployment of sensors using genetic algorithms and also applying the Internet of Things (IoT) in regards of coverage, localization network lifetime and connectivity that allowed to maximization on data collection. Mnasri et al. [8] used hybrid many-objective optimization algorithms for the purpose. This approach can be an application in terms of Agriculture 4.0. In this context, Oruma [9] presents agriculture 4.0 to tackle climate change, growing world population and environmental challenges with a particular focus on crop production. Other examples are decision support system for livestock [10] and smart irrigation systems for improving the sustainability of agriculture [11].

III. Materials and Methods

The mathematical model is essentially divided into two parts, or two objective functions. One is related to the path of the pesticide after application and its impact on environmental, thus it covers the life cycle of the pesticide. The second is related to the minimum phytopharmaceutical dose required, considering the above-described parameters.

A. Part A – Simulation of pesticide path after application

The first part (A) consists of creating an algorithm capable of simulating the behaviour of a pesticide over time. Starting at the initial point of application, up to the remaining theoretical quantification of it at the end of a defined period.

Such mathematical model is proposed by Tang [5]. This model provides a set of equations that simulate the course of a pesticide from its application to the end of life cycle. Figure 1 illustrates the general scheme of the mass flow and the different fractions in the respective path of a pesticide after application described within the model.

Three variables are defined, the pesticide fraction that leached to the aquatic environment, f_{water}, the fraction of the dispersion by the field according to the area, f_{drift} and finally the fraction that really comes into contact with the plants, f_{leaf}. The combination of these three fractions represents 100% of the applied phytopharmaceutical. It is then necessary to define each expression. The fraction of phytopharmaceuticals that is leached in the water is defined by the Equations 1 to 7.

$$\begin{cases} 0, & t = 0 \\ f_{wa,t} = (f_{ads,t} - f_{des,t}) + f_{wa.t-1}) \cdot (k_s.t), & t > 0 \end{cases} \quad (1)$$

Where $f_{ads,t}$ and $f_{des,t}$ represent the fractions of adsorption and desorption on the day *t* and k_{wa} *and* k_{des} the constants of the process in day^{-1}, respectively.

For formulations of liquid pesticides, $k_s \cdot t = 1$.

The adsorbed fraction is given by Equation (2).

$$f_{ads,t} = 1 - e^{-k_{wa}w_t} \quad (2)$$

For the calculation of k_{wa}, the support Equations (3) to (5) provided by Tang [5] were used:

$$k_{wa} = d \cdot \rho \cdot 2 \cdot k_{des} \cdot \frac{k_f}{D} \quad (3)$$

$$k_f = oc.\frac{k_{oc}}{100} \quad (4)$$

$$k_{des} = 0.0339 \; with \; S > 1000 \quad (5)$$

Where, d is the thickness of the surface soil layer (m), ρ the dry soil density (ton/m^3), k_{des} is the constant of solubility (S) of water above 1000 (g/m^3). k_f is calculated in Equation (3) with oc describing carbon content in the organic form in percentage in the type of soil and k_{oc} is the adsorption coefficient of carbon in organic form (ml/g), and lastly, $w_t = 2.34$ is the dissociation constant of the glyphosate calculated at 25°C of the pesticide [7]. It should be noted that the value of k_f represents the soil adsorption coefficient for an isothermal *Freundlich*. This value can be for glyphosate is $k_f = 226.3$ [7].

The desorption behaviour is given by Equation 6:

$$f_{des,t} = (1 - e^{-k_{des}}) \cdot f_{ads,t} \quad (6)$$

Where $f_{ads,t}$ is calculated by Equation 2.

The fraction from the process by volatilization, degradation, leaching and adsorption at the end of 30 days of application, $f_{i,t}$ is given by Equation (7):

$$f_{i,t} = \left(1 - e^{-k_i w_t} + f_{i,t-1}\right) \quad (7)$$

The fraction of the dispersion by the field according to the area, f_{drift} is given by Equation (8):

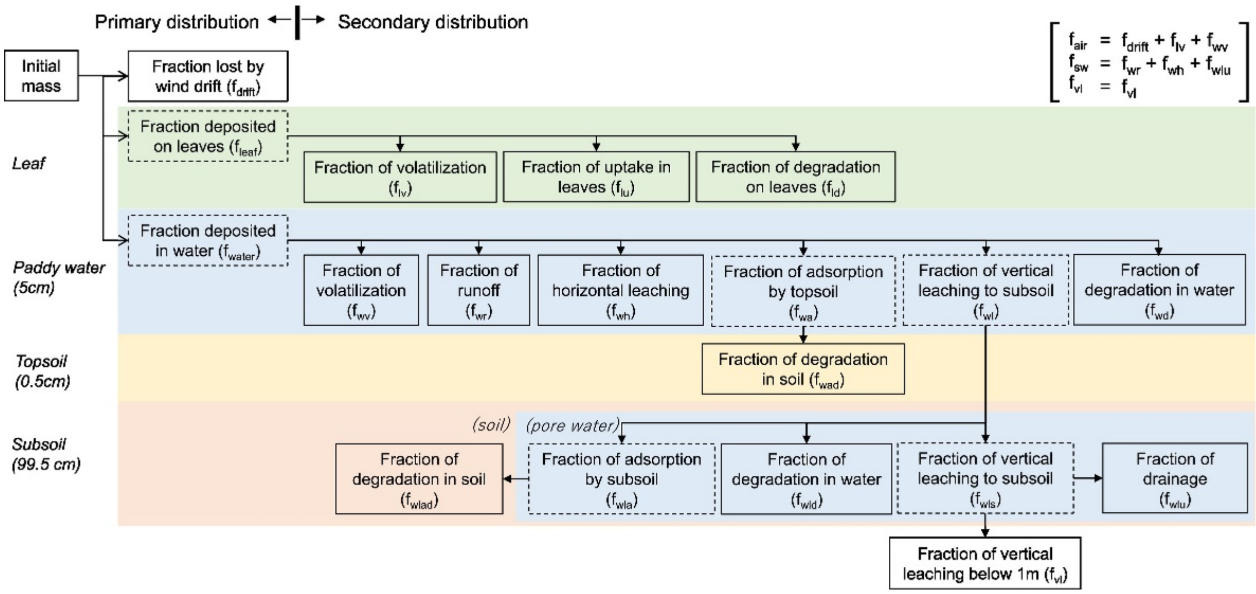

Fig. 1- General scheme of the mass flow and the different fractions in the respective path of a pesticide after application [5].

$$f_{drift} = \frac{1}{n}\sum \binom{i=n}{1} f(x_i) \quad (8)$$

$$n = \frac{\sqrt{A}}{W} \quad (9)$$

$$x_i = W \cdot i - \frac{W}{2} \quad (10)$$

Where $\sqrt{A}$ is the length of the agricultural field (m), W the width of the field (m) and x_i the distance between the field centre of mass and the outer limits of the field (m).

Knowing these variables, it is possible to determine the fractions for each component in the life cycle of the pesticide by Equation (11):

$$f_{total} = f_{drift} + f_{leaf} + f_{water} \quad (11)$$

The fraction that really comes into contact with the plants, f_{leaf} can be directly calculated by Equation (12):

$$f_{leaf} = f_{total} - f_{drift} - f_{water} \quad (12)$$

The value can be obtained for each application varying in a dynamic way due to the day and dimensions of the field where the environmental impact and the presence of the pesticide, ranging from the moment of application up to a maximum of 30 days. Thus, this result provides the simulation of the pesticide applied for protective purposes on the plant and how much was actually lost and dispersed by the environment.

B. Part B - Minimum phytopharmaceutical dose

For the second part of the model, an objective function capable of quantifying the minimum phytopharmaceutical dose required according to the defined variables is presented. Equations employed in this part of the model were developed by Holterman [12]. Equations consider the atmospheric variables such as the wind speed, F_{wj}, the temperature F_{Tj}, the density of the orchard canopy, F_N, the quantities of pesticide applied q_{j0} and F_f for fan speed setting. Each of these variables are described in the following equations.

The determination of the influence of the direction in the dispersion of a phytopharmaceutical is given by Equation (13):

$$s = \frac{x}{\cos(\theta)} \quad (13)$$

Where x is the perpendicular distance (m) and $\cos(\theta)$ varying between $\theta > 90°$ and $\theta < -90°$.

The graphic representation of the Equation (13) is shown in Figure 2.

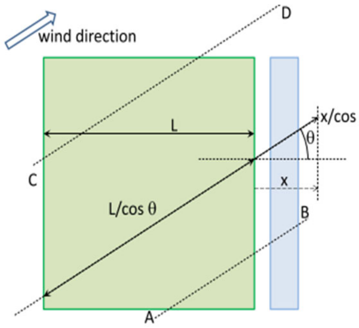

Fig. 2 - Representation of pesticide dispersion along the field due to distance. [12]

Equation (14) describes the temperature influence:

$$F_{Tj} = 1 + b_{1j}(T - T_0) + b_{2j}(T - T_0)^2 \quad (14)$$

Where b_{1j} is given by the expression $\frac{1}{°C}$, and b_{2j} is given by $\frac{1}{°C^2}$, T is the temperature during pesticide application (ºC) and T_0 as a reference temperature (ºC).

The density of the canopy described by F_{Nj} is simulated by Equation (15):

$$\beta = 1 - e^{(-a_0 \sin \pi v)^{a_4}} \quad (15)$$

This function β defines the variation of canopy density over a year represented in Figure 3:

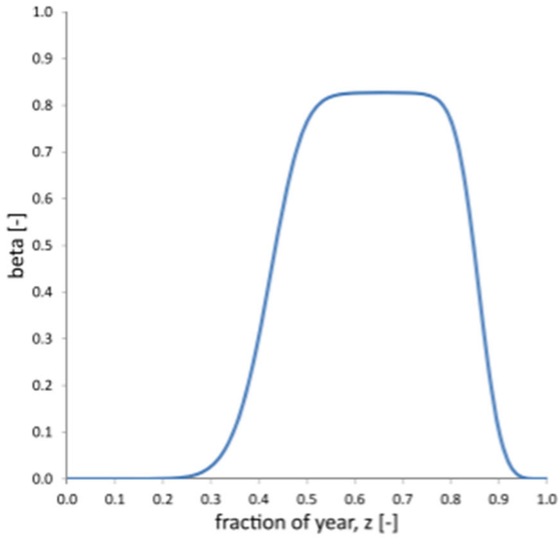

Fig. 3 - Representation of the density of treetops according to the part of the year given by *z*. [12]

This function was simplified. The 12 months of the year were divided by 10 so that there is an approximate correspondence of each scale value in months of the year.

Then there was approximated each value given by *z* corresponding to one month of the year and its corresponding

β value. These relationships are described in the code of the created program.

The fan setting was defined by $F_f = 0{,}85$, considering that is an average value.

For the calculation of q_{j0}, that is, the initial quantities of phytopharmaceutical, the Equation (16) was used:

$$q_{j0} = Q_{min} \cdot \left(\frac{a \cdot i}{ha}\right) \quad (16)$$

Equation 16 was adapted from concentration equation given by: $g \cdot \left(\frac{a.i}{ha}\right)$ proposed by Felix [2], where Q_{min} is the amount of pesticide recommended by the phytopharmaceutical supplier with $Q_{min} = \frac{L}{ha}$, $a \cdot i$ is the "Active Ingredient", that is, the active substance present in the type of pesticide and ha, is the area (ha). To note that the value of $a \cdot i = \frac{360g}{L}$. This value is referring to the glyphosate [6].

F_{wj} calculates the impact of wind speed, defined by Equation (17):

$$F_{wj} = e^{-a_{1j}(w-w_0)-a_{2j}(w-w_0)^2} \quad (17)$$

Where a_{1j} *and* a_{2j} are constants, w is the wind speed (m s^{-1}), w_0 is a user-defined reference wind speed. The function F_{wj} assumes a value of 1 when $w = w_0$, so the wind speed can be fixed at a constant value, simplifying the value for 1. Thus, the impact on results is given by the inlet angle of the wind and not by speed.

Finally, knowing the value of each variable, the ideal dose, q_j, calculated according to the initial concentration and the factors involved above, is given by Equation (18).

$$q_j = q_{j0} \cdot F_{wj} \cdot F_{Tj} \cdot F_{Nj} \cdot F_{fj} \quad (18)$$

q_j is expressed in $\mathrm{g.L^{-1}}$, but for simplification purposes, the final value is converted to be given in L.

IV. COMPUTATIONAL TOOL

Analysis of the existing bibliography for the creation of decision support tools for the application of a phytopharmaceutical resulted in the choice of a set of equations that define variables in the process of application of such products.

With these equations previously defined, it was possible to build a program capable of evaluating data inputs in the form of variables. This program is essentially divided into two parts, that is, two objective functions. The first capable of simulating the behaviour of the application of a phytopharmaceutical along and up to a 30-day limit. The second part is capable of simulating the exact quantities of phytopharmaceuticals to be applied, taking into account the applied doses, as well as the environmental factors involved. The program code is attached.

This program was developed in Python, as this language is versatile and allows you to make modifications capable of improving the program created.

The first part of the program simulates the dispersion of a pesticide, and consequently the life cycle in the environment, providing a view of behaviour when applied the phytopharmaceutical, that is, how much it was used to create a protective effect on plants, or ended up dispersed by air or in water courses.

The second part can give an adjusted response taking into account atmospheric conditions such as temperature, wind and applied phytopharmaceutical quantities. Gathering both objective functions, allows to calculate the exact quantities to be applied, by making an adjustment according to the input variables, providing a decision-making support tool for the optimized application of phytopharmaceutical.

V. CASE STUDY

A case study is proposed to verify the applicability of the tool developed for the correct amount of phytopharmaceutical to be applied, concerning the environmental conditions at the time of application. The case study was developed with a local farmer. This specific farmer has orchards of chestnut, olive trees and almond trees. The olive trees orchard was selected for the case study since it requires permanent attention all year round and it is harvested between November and January. Two fields are cultivated. One with 3.5 ha with almond trees with 5 m distance between tree rows. The other field has 2.5 ha with olive trees with 7 m distance between tree rows. A representation of the olive trees field is shown in Figure 4.

Fig. 4 – Case study - olive trees field.

August is one of the most critical months as phytopharmaceuticals should be applied to avoid weeds. The pesticide utilized is glyphosate with the application distance ranging from 10 to 50 cm at a canopy level. The air temperature varies between 20°C and 40 °C in summer in the orchard location. Wind speed must be low, ranging around 2 m s^{-1} . Wind direction θ varies between 30° to 60°. For calculations, an average air temperature of 30 ºC and an average wind direction of 45° were set.

However, conditions without wind are desirable. Thus, these environmental conditions were also considered, performing the required code adjustments.

When the phytopharmaceutical is applied, a medium velocity is used in fan setting. The recommended initial applied dose is 2 L/ha.

VI. ANALYSIS AND DISCUSSION OF RESULTS

Preliminary results obtained using the computational decision-making support tool for the optimized application of phytopharmaceuticals shown that for the conditions above described, the initial dose calculated is 12.55 L/ha for the field with 2.5 ha when wind speed of 2 m s^{-1} , temperature of 30 °C, and a wind direction of 45° are considered. This results highlights the large impact of the wind factor and its direction. However, the decision tool is also able to optimize the necessary amount of phytopharmaceuticals in the ideal conditions, reducing to 4.88 L/ha, and when there is no wind it predicts an amount of 0.8 L/ha. Analysing the results it might seem odd that it is required such amount for a small field. However, it must be considered a larger amount of phytopharmaceuticals must be applied to compensate the part that might be dispersed and lost. With a larger field, much more quantity of phytopharmaceuticals would have stayed in the field after application, and not get dispersed out of the field. In this case, the overall amount needed is reduced. Although, these predictions require to be validated with specific field tests to access the prediction accuracy of the computational decision-making support tool for the optimized application of phytopharmaceuticals.

VII. CONCLUSIONS

A multi-objective decision-making support tool for the optimized application of phytopharmaceuticals is proposed. The model is composed by mathematical formulations related to the path of the pesticide after application and its impact on environmental and to the minimum phytopharmaceutical dose required, taking into account the above described parameters. Gathering both impacts can provide the minimization of the pesticide amount required with gains for environment and farmer.

Some future ideas can be proposed to improve the model. Using Machine Learning, the system can be trained to provide more reliable answers with adjustment to real conditions. Another proposal is the possibility of introducing new variables to improve the robustness of the model, making it more capable of simulating the actual real conditions.

The program is developed for the use of glyphosate, however, this is not the only pesticide in use. So, adapting the model to other type of phytopharmaceuticals would also be pertinent.

It will be interesting from the user's point of view to simplify some of the input variables, such as the capacity of the program to collect direct information of sensors such as dispersers, or wind speed that can be felt in real time and do the respective adjustment.

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