Math. Model. Nat. Phenom. 19 (2024) 22
https://doi.org/10.1051/mmnp/2024021

Mathematical Modelling of Natural Phenomena
www.mmnp-journal.org

COMPARISON OF TWO APPROACHES FOR SOLVING A FUZZY SYSTEM DESCRIBING THE DEGRADATION KINETICS OF PESTICIDES IN PLANT UPTAKE MODELS

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Abstract. Chemical control in agriculture includes the use of chemical agents whose concentrations in the harvest products decrease over time. We analyze mathematically the decrease of pesticide residues in potato tubers, and estimate the involved parameters to predict the evolution of pesticide residual after the last spraying. First, we propose and solve a fuzzy initial value problem (FIVP) associated with a fuzzy differential equations system modeling the pesticide concentration in potato tubers. Second, we apply our model in a real situation, where the evolution of the concentration of chemicals is required, by considering two approaches. In the first one, based on a small set of field data, we use a polynomial regression (LOESS) to input new data and estimate the parameters involved in the FIVP and thus, we determinate the evolution of the concentration of the thiamethoxam, a pesticide used on potato crops. In the second approach, we design a Takagi–Sugeno–Kang model to approximate the degradation of thiamethoxam concentration, by defining a set of fuzzy inference rules based on the data provided by LOESS regression. These two approaches show a similar and good behavior, even having few fuzzy data. Our analysis can be applied in a large class of dynamical systems.

Mathematics Subject Classification. 34A07, 03E72, 03B52, 62G08, 92B10, 93C42.

Received August 12, 2024. Accepted November 20, 2024.

1. Introduction

The use of pesticides in agricultural crops is fundamental to the chemical control of pest and disease, which translates into pesticide application by the grower on the crop through spraying. One of the most important crops in the global production, after sugarcane, corn, wheat, rice and oil palm fruit, is the potato (Solanum tuberosum) [1], a native product of the Andes region of South America, with more than five thousand edible varieties [2]. One of the main pests in the potato crop is the potato white worm (Premnotrypes Vorax), for which the common pesticides used in its control generally combine the action of two active ingredients: thiamethoxam (Neonicotinoid) and lambda-cyhalothrin (Synthetic pyrethroid). The thiamethoxam is a systemic insecticide that inhibits nicotinic acetylcholine receptors [3], while lambda-cyhalothrin is a non-systemic insecticide that interferes with the sodium channel [4]. These chemicals produce a loss of control, paralysis and afterwards, the death of the pest.

Keywords and phrases: Pesticide concentration in potato, parameter estimation, fuzzy ordinary differential equations, Takagi–Sugeno–Kang model.

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Analysis of chemical residues in the harvest products (in this case, the potato tuber) is a relevant problem to study the quality and suitability of the product for human consumption, considering the parameters established by the Food and Agriculture Organization of the United Nations (FAO) and the World Health Organization (WHO). Some statistical analysis about this problem has been presented in [5, 6], and [7]. In [5] the author considered an exponential decreasing behavior of the pesticide concentration in potato and in soil without considering external agents or processes that affect the dynamics; on the other hand, in [6, 7], considering complex open field conditions including multiple processes of pesticide uptake and elimination by plants, the authors established a system of ordinary differential equations for modeling pesticide concentration in potato using the results of [8] and [9].

In this work, we propose the use of fuzzy mathematical models to describe the concentration behavior of pesticides in potato tubers $C_p(t)$ considering the nondeterministic nature of the data obtained in field, as well as the imprecision, vagueness, subjectivity, fuzziness and uncertainty involved. First, we use the theory of fuzzy ordinary differential equations (ODE) [10–18] to describe the decrease of pesticide concentration in potato tubers considering a fuzzy version of the crisp model proposed in [7]. In this case, we consider that the initial concentration of the pesticide in the soil and in the potato tubers are fuzzy numbers which correspond to a more realistic scenario; indeed, as a case study we analyze the residual of thiamethoxam in potato by using field data from a potato crop of Santander, Colombia, and information in the literature [5, 7, 19], to estimate and to establish the degradation, dilution and diffusion parameters of thiamethoxam involved in the model, by using some statistical tools, namely, local polynomial regressions and nonlinear least squares. The second aim of this paper is to design a model based on fuzzy inference rules of Takagi–Sugeno–Kang type (TSK) [20] to describe the time variation of the chemical concentration ($\Delta C_p(t)$) to finally interpolate the concentration curve of pesticide in potato tubers. We compare these two approaches and as result, we conclude that they have a similar behavior. Both approaches could be used as good tools for modeling the concentration of other pesticides or chemicals in potato tubers.

This current study was carried out in order to introduce and develop a mathematical tool to deal with a realistic agricultural problem. In Section 2, we propose and solve the general Fuzzy ODE system expressing the solution in terms of the involved parameters. In Section 3, we analyze the determination of the parameters in a specific real situation, that is, considering data related to the thiamethoxam concentration in potato. Estimating the set of parameters, we are able to determinate explicitly the concentration of the pesticide over time. In Section 4, we design a TSK model to approximate the variation of the concentration of thiamethoxam, as an alternative approach. Finally, we compare these two approaches, showing a quite reasonable approximation in its behavior, even having a minimum amount of fuzzy data.

2. Mathematical model

Considering the nondeterministic nature of the initial concentration data of pesticides in potato tubers, as well as the fuzzy nature of the degradation and diffusion parameters (how it actually happens), we propose a mathematical model for describing the evolution of the pesticide concentration in potato $C_p(t)$, via the following fuzzy ordinary differential equations system:

$$\begin{cases} C_p'(t) = & k_{s\to p}C_s(t) + (-1)[k_{p\to s} + k_{\text{growth},p} + k_{\text{deg},p}]C_p(t), \\ C_s'(t) = & -k_{\text{deg},s}C_s(t), \\ C_p(0) = & C_{p_0}, \\ C_s(0) = & C_{s_0}, \end{cases} \tag{2.1}$$

where $C_p(t)$ and $C_s(t)$ are fuzzy functions representing the pesticide concentrations in potato tubers and soil respectively, with their respective pesticide degradation rates $k_{\text{deg},p}$ and $k_{\text{deg},s}$. In addition, $k_{s\to p}$ and $k_{p\to s}$ are the rates of soil-to-potato uptake and potato-to-soil removal of pesticide by diffusion, and $k_{\text{growth},p}$ denotes the growth rate of potato. The terms C_{p_0} and C_{s_0} are the initial data which are assumed elements of $\mathcal{F}$ (space of the fuzzy numbers of $\mathbb{R}$ with α-levels being compact intervals in $\mathbb{R}$). System (2.1) corresponds to a fuzzy version of the differential system proposed by [6] and [7]. Thus, the first key element in the description of the fuzzy system (2.1), is the sense of the derivative $C_p'(t)$. Following [10–13, 17, 18] we use the concept of the generalized Hukuhara derivative (gH-derivative for short). We recall that a fuzzy function $f:[0,T]\to\mathcal{F}$ is said gH-differentiable in $t\in[0,T]$, if there exists $f'_{gH}(t)\in\mathcal{F}$ such that

$$f'_{gH}(t)=\lim_{h\to 0}\frac{1}{h}\left[f(t+h)\ominus_{gH} f(t)\right], \tag{2.2}$$

where $\ominus_{gH}$ is the Hukuhara generalized difference between fuzzy numbers, that is, for $u,v,z\in\mathcal{F}$, the gH-difference $u\ominus_{gH} v=z$, if, and only if, $u=v+z$ or $v=u+(-1)z$ (see [10, 13]). If $u=v+z$, then z is called the Hukuhara difference between u and v, and it is denoted by $u\ominus v$. Taking into account the definition of the difference $\ominus_{gH}$, from (2.2), we have two cases, namely, (i)–gH derivative and (ii)–gH derivative. We say that f is (i)–gH differentiable if the Hukuhara differences $f(t+h)\ominus f(t)$, $f(t)\ominus f(t-h)$ exist and

$$f'_{gH}(t)=\lim_{h\to 0^+}\frac{1}{h}\left[f(t+h)\ominus f(t)\right]=\lim_{h\to 0^+}\frac{1}{h}\left[f(t)\ominus f(t-h)\right],$$

and f is (ii)–gH differentiable if the Hukuhara differences $f(t)\ominus f(t+h)$, $f(t-h)\ominus f(t)$ exist and

$$f'_{gH}(t)=\lim_{h\to 0^+}\frac{1}{-h}\left[f(t)\ominus f(t+h)\right]=\lim_{h\to 0^+}\frac{1}{-h}\left[f(t-h)\ominus f(t)\right].$$

In order to solve (2.1), taking into account that (2.1) is a (semi) decoupled system, we first solve $(2.1)_{2,4}$, and then we replace $C_s(t)$ in $(2.1)_{1,3}$ and solve it to get $C_p(t)$. This procedure is done in next subsections.

2.1. Pesticide concentration in soil

Considering the initial pesticide concentration in soil C_{s_0} as a fuzzy number (for simplicity, a triangular fuzzy number), we first solve the fuzzy initial value problem

$$\begin{cases} C_s'(t) &= -k_{\mathrm{deg},s}C_s(t),\\ C_s(0) &= C_{s_0}, \end{cases} \tag{2.3}$$

where, as said, $C_s(t)$ represents the pesticide concentration at time t, and $k_{\mathrm{deg},s}$ is the pesticide degradation rate in soil. We have two cases, depending on the sense of the kind of gH-derivative. Indeed, if $C_s(t)$ is (i)–gH differentiable, then the α-levels of $C_s'(t)$ are given by
$[{C_s}'(t)]^\alpha=[\underline{C_s^{\alpha\prime}(t)},\overline{C_s^{\alpha\prime}(t)}]=[-k_{\mathrm{deg},s}\overline{C_s^\alpha(t)},-k_{\mathrm{deg},s}\underline{C_s^\alpha(t)}]$. Here, $[{C_s}'(t)]^\alpha=[\underline{C_s^{\alpha\prime}(t)},\overline{C_s^{\alpha\prime}(t)}]$ denotes the α-levels of the (i)–gH derivative of $C_s(t)$, which means that $\underline{C_s^{\alpha\prime}(t)}$ is the derivative of $\underline{C_s^\alpha(t)}$ and $\overline{C_s^{\alpha\prime}(t)}$ is the derivative of $\overline{C_s^\alpha(t)}$. Therefore, the (i)–gH solution of (2.3) in terms of its α-levels is given by

$$[C_s(t)]^\alpha=\frac{1}{2}\left[\left(\underline{C_{s_0}^\alpha}+\overline{C_{s_0}^\alpha}\right)\mathrm{e}^{-k_{\mathrm{deg},s}t}-\left(\overline{C_{s_0}^\alpha}-\underline{C_{s_0}^\alpha}\right)\mathrm{e}^{k_{\mathrm{deg},s}t},(\underline{C_{s_0}^\alpha}+\overline{C_{s_0}^\alpha})\mathrm{e}^{-k_{\mathrm{deg},s}t}+(\overline{C_{s_0}^\alpha}-\underline{C_{s_0}^\alpha})\mathrm{e}^{k_{\mathrm{deg},s}t}\right]. \tag{2.4}$$

On the other hand, if $C_s(t)$ is (ii)–gH differentiable we have that
$[{C_s}'(t)]^\alpha=[\overline{C_s^{\alpha\prime}(t)},\underline{C_s^{\alpha\prime}(t)}]=[-k_{\mathrm{deg},s}\overline{C_s^\alpha(t)},-k_{\mathrm{deg},s}\underline{C_s^\alpha(t)}]$; then the (ii)–gH solution of (2.3) is given by

$$[C_s(t)]^\alpha=\left[\underline{C_{s_0}^\alpha}\mathrm{e}^{-k_{\mathrm{deg},s}t},\overline{C_{s_0}^\alpha}\mathrm{e}^{-k_{\mathrm{deg},s}t}\right]. \tag{2.5}$$

2.2. Pesticide concentration in potato tuber

We replace the fuzzy function $C_s(t)$, obtained in Section 2.1, in $(2.1)_1$, and then we solve the FIVP $(2.1)_{1,3}$ to get $C_p(t)$. We consider $k_{s\to p}, \lambda = -[k_{p\to s} + k_{\text{growth},p} + k_{\text{deg},p}] \in \mathbb{R}^-$ and $k_{\text{deg},s} \in \mathbb{R}^+$. Let $[C_s(t)]^\alpha = [\underline{C_s^\alpha(t)}, \overline{C_s^\alpha(t)}]$ and $[C_p(t)]^\alpha = [\underline{C_p^\alpha(t)}, \overline{C_p^\alpha(t)}]$ the α-levels of the fuzzy functions $C_s(t)$ (see Sect. 2.1) and $C_p(t)$ respectively, with initial concentration data $[C_s(0)]^\alpha = [\underline{C_{s_0}^\alpha}, \overline{C_{s_0}^\alpha}]$ and $[C_p(0)]^\alpha = [\underline{C_{p_0}^\alpha}, \overline{C_{p_0}^\alpha}]$. We have that

$$\begin{aligned}
[k_{s\to p}C_s(t) + \lambda C_p(t)]^\alpha &= k_{s\to p}[C_s(t)]^\alpha + \lambda[C_p(t)]^\alpha\\
&= [k_{s\to p}\overline{C_s^\alpha(t)}, k_{s\to p}\underline{C_s^\alpha(t)}] + [\lambda\overline{C_p^\alpha(t)}, \lambda\underline{C_p^\alpha(t)}]\\
&= [k_{s\to p}\overline{C_s^\alpha(t)} + \lambda\overline{C_p^\alpha(t)}, k_{s\to p}\underline{C_s^\alpha(t)} + \lambda\underline{C_p^\alpha(t)}].
\end{aligned}$$

Thus, if $C_p(t)$ is (i)–gH differentiable, we have that

$$[C'(t)]^\alpha = [\underline{C_p^{\alpha\prime}(t)}, \overline{C_p^{\alpha\prime}(t)}] = [k_{s\to p}\overline{C_s^\alpha(t)} + \lambda\overline{C_p^\alpha(t)}, k_{s\to p}\underline{C_s^\alpha(t)} + \lambda\underline{C_p^\alpha(t)}]. \tag{2.6}$$

On the other hand, if $C_p(t)$ is (ii)–gH differentiable, the α-levels of $C_p'(t)$ are such that

$$[C'(t)]^\alpha = [\overline{C_p^{\alpha\prime}(t)}, \underline{C_p^{\alpha\prime}(t)}] = [k_{s\to p}\overline{C_s^\alpha(t)} + \lambda\overline{C_p^\alpha(t)}, k_{s\to p}\underline{C_s^\alpha(t)} + \lambda\underline{C_p^\alpha(t)}]. \tag{2.7}$$

In this point it is important to observe that for replacing the α-levels of $C_s(t)$, we need to consider the corresponding two cases which coming from the sense of the gH derivative in $C_s'(t)$. This implies that in total, we have four possible solutions, namely (i)–(i)–gH solution, (i)–(ii)–gH solution, (ii)–(i)–gH solution and (ii)–(ii)–gH solution according to the derivative cases. Below we describe each one of them.

2.2.1. (i)–(i)–gH derivative

In this case, we consider that $C_p(t)$ and $C_s(t)$ are (i)–gH differentiable; that is, $C_p'(t)$ is as in (2.6) and $C_s(t)$ is given by (2.4). Then, the fuzzy initial value problem (2.1) is equivalent to solve the following system of ODE:

$$\begin{cases}
\underline{C_p^{\alpha\prime}(t)} = \frac{k_{s\to p}}{2}\left[\left(\underline{C_{s_0}^\alpha} + \overline{C_{s_0}^\alpha}\right)e^{-k_{\text{deg},s}t} + \left(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha}\right)e^{k_{\text{deg},s}t}\right] + \lambda\overline{C_p^\alpha(t)},\\
\overline{C_p^{\alpha\prime}(t)} = \frac{k_{s\to p}}{2}\left[\left(\underline{C_{s_0}^\alpha} + \overline{C_{s_0}^\alpha}\right)e^{-k_{\text{deg},s}t} - \left(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha}\right)e^{k_{\text{deg},s}t}\right] + \lambda\underline{C_p^\alpha(t)},\\
\underline{C_p^\alpha(0)} = \underline{C_{p_0}^\alpha}, \ \overline{C_p^\alpha(0)} = \overline{C_{p_0}^\alpha},\\
\underline{C_s^\alpha(0)} = \underline{C_{s_0}^\alpha}, \ \overline{C_s^\alpha(0)} = \overline{C_{s_0}^\alpha},
\end{cases} \quad \alpha \in [0,1], \tag{2.8}$$

thus, the solution of (2.1) (the (i)–(i)–gH solution) in terms of its α-levels is given by

$$\begin{cases}
\underline{C_p^\alpha(t)} = C_1e^{\lambda t} - C_2e^{-\lambda t} + \frac{k_{s\to p}}{2(\lambda + k_{\text{deg},s})}\left(-(\overline{C_{s_0}^\alpha} + \underline{C_{s_0}^\alpha})e^{-k_{\text{deg},s}t} + (\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha})e^{k_{\text{deg},s}t}\right),\\
\overline{C_p^\alpha(t)} = C_1e^{\lambda t} + C_2e^{-\lambda t} - \frac{k_{s\to p}}{2(\lambda + k_{\text{deg},s})}\left((\overline{C_{s_0}^\alpha} + \underline{C_{s_0}^\alpha})e^{-k_{\text{deg},s}t} + (\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha})e^{k_{\text{deg},s}t}\right),
\end{cases} \quad \alpha \in [0,1],$$

where,

$$\begin{cases}
C_1 = \frac{1}{2}\left(\underline{C_{p_0}^\alpha} + \overline{C_{p_0}^\alpha} + \frac{k_{s\to p}}{(\lambda + k_{\text{deg},s})}(\underline{C_{s_0}^\alpha} + \overline{C_{s_0}^\alpha})\right),\\
C_2 = \frac{1}{2}\left(\overline{C_{p_0}^\alpha} - \underline{C_{p_0}^\alpha} + \frac{k_{s\to p}}{(\lambda + k_{\text{deg},s})}(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha})\right),
\end{cases} \quad \alpha \in [0,1].$$

2.2.2. (i)–(ii)–gH derivative

In the second case, we consider that $C_p(t)$ is (i)–gH differentiable and $C_s(t)$ is (ii)–gH differentiable; that is, $C_p'(t)$ is as in (2.6) and $C_s(t)$ is given by (2.5), obtaining the following system of ODE:

$$\begin{cases} \underline{C_p^\alpha}'(t) = k_{s\to p}\overline{C_{s_0}^\alpha}\mathrm{e}^{-k_{\mathrm{deg},s}t} + \lambda\overline{C_p^\alpha(t)}, \\ \overline{C_p^\alpha}'(t) = k_{s\to p}\underline{C_{s_0}^\alpha}\mathrm{e}^{-k_{\mathrm{deg},s}t} + \lambda\underline{C_p^\alpha(t)}, \\ \underline{C_p^\alpha}(0) = \underline{C_{p_0}^\alpha},\ \overline{C_p^\alpha}(0) = \overline{C_{p_0}^\alpha}, \\ \underline{C_s^\alpha}(0) = \underline{C_{s_0}^\alpha},\ \overline{C_s^\alpha}(0) = \overline{C_{s_0}^\alpha}, \end{cases} \alpha \in [0,1]\,, \tag{2.9}$$

thus, the solution of (2.1) (the (i)–(ii)–gH solution) is given by

$$\begin{cases} \underline{C_p^\alpha(t)} = C_1\mathrm{e}^{\lambda t} - C_2\mathrm{e}^{-\lambda t} + \frac{k_{s\to p}\overline{C_{s_0}^\alpha}k_{\mathrm{deg},s} - \lambda\underline{C_{s_0}^\alpha}k_{s\to p}}{\lambda^2 - k_{\mathrm{deg},s}^2}\mathrm{e}^{-k_{\mathrm{deg},s}t}, \\ \overline{C_p^\alpha(t)} = C_1\mathrm{e}^{\lambda t} + C_2\mathrm{e}^{-\lambda t} + \frac{k_{s\to p}\underline{C_{s_0}^\alpha}k_{\mathrm{deg},s} - \lambda\overline{C_{s_0}^\alpha}k_{s\to p}}{\lambda^2 - k_{\mathrm{deg},s}^2}\mathrm{e}^{-k_{\mathrm{deg},s}t}, \end{cases} \alpha \in [0,1]\,,$$

where,

$$\begin{cases} C_1 = \frac{1}{2}\left(\underline{C_{p_0}^\alpha} + \overline{C_{p_0}^\alpha} - \frac{k_{s\to p}(k_{\mathrm{deg},s}-\lambda)}{\lambda^2 - k_{\mathrm{deg},s}^2}(\overline{C_{s_0}^\alpha} + \underline{C_{s_0}^\alpha})\right), \\ C_2 = \frac{1}{2}\left(\overline{C_{p_0}^\alpha} - \underline{C_{p_0}^\alpha} + \frac{k_{s\to p}(k_{\mathrm{deg},s}+\lambda)}{\lambda^2 - k_{\mathrm{deg},s}^2}(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha})\right), \end{cases} \alpha \in [0,1]\,.$$

2.2.3. (ii)–(i)–gH derivative

In the third case, we consider that $C_p(t)$ is (ii)–gH differentiable and $C_s(t)$ is (i)–gH differentiable; that is, $C_p'(t)$ and $C_s(t)$ are given as in (2.7) and (2.4), respectively. Then we obtain the following system of ODE:

$$\begin{cases} \underline{C_p^\alpha}'(t) = \frac{k_{s\to p}}{2}\left[\left(\underline{C_{s_0}^\alpha} + \overline{C_{s_0}^\alpha}\right)\mathrm{e}^{-k_{\mathrm{deg},s}t} - \left(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha}\right)\mathrm{e}^{k_{\mathrm{deg},s}t}\right] + \lambda\underline{C_p^\alpha(t)}, \\ \overline{C_p^\alpha}'(t) = \frac{k_{s\to p}}{2}\left[\left(\underline{C_{s_0}^\alpha} + \overline{C_{s_0}^\alpha}\right)\mathrm{e}^{-k_{\mathrm{deg},s}t} + \left(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha}\right)\mathrm{e}^{k_{\mathrm{deg},s}t}\right] + \lambda\overline{C_p^\alpha(t)}, \\ \underline{C_p^\alpha}(0) = \underline{C_{p_0}^\alpha},\ \overline{C_p^\alpha}(0) = \overline{C_{p_0}^\alpha}, \\ \underline{C_s^\alpha}(0) = \underline{C_{s_0}^\alpha},\ \overline{C_s^\alpha}(0) = \overline{C_{s_0}^\alpha}, \end{cases} \alpha \in [0,1]\,. \tag{2.10}$$

Solving (2.10) we find that the solution of (2.1) (the (ii)–(i)–gH solution) is given by

$$\begin{cases} \underline{C_p^\alpha(t)} = C_1\mathrm{e}^{\lambda t} + \frac{k_{s\to p}}{2(-k_{\mathrm{deg},s}-\lambda)}\left(\overline{C_{s_0}^\alpha} + \underline{C_{s_0}^\alpha}\right)\mathrm{e}^{-k_{\mathrm{deg},s}t} - \frac{k_{s\to p}}{2(k_{\mathrm{deg},s}-\lambda)}\left(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha}\right)\mathrm{e}^{k_{\mathrm{deg},s}t}, \\ \overline{C_p^\alpha(t)} = C_2\mathrm{e}^{\lambda t} + \frac{k_{s\to p}}{2(-k_{\mathrm{deg},s}-\lambda)}\left(\overline{C_{s_0}^\alpha} + \underline{C_{s_0}^\alpha}\right)\mathrm{e}^{-k_{\mathrm{deg},s}t} + \frac{k_{s\to p}}{2(k_{\mathrm{deg},s}-\lambda)}\left(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha}\right)\mathrm{e}^{k_{\mathrm{deg},s}t}, \end{cases} \alpha \in [0,1]\,,$$

where,

$$\begin{cases} C_1 = \underline{C_{p_0}^\alpha} - \frac{k_{s\to p}}{2(-k_{\mathrm{deg},s}-\lambda)}\left(\overline{C_{s_0}^\alpha} + \underline{C_{s_0}^\alpha}\right) + \frac{k_{s\to p}}{2(k_{\mathrm{deg},s}-\lambda)}\left(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha}\right), \\ C_2 = \overline{C_{p_0}^\alpha} - \frac{k_{s\to p}}{2(-k_{\mathrm{deg},s}-\lambda)}\left(\overline{C_{s_0}^\alpha} + \underline{C_{s_0}^\alpha}\right) - \frac{k_{s\to p}}{2(k_{\mathrm{deg},s}-\lambda)}\left(\overline{C_{s_0}^\alpha} - \underline{C_{s_0}^\alpha}\right), \end{cases} \alpha \in [0,1]\,.$$

TABLE 1. Data obtained in laboratory.

Time (days)	Concentration (μg kg^{-1})
0	16.39
3	11.72
10	8.15

2.2.4. (ii)–(ii)–gH derivative

In the fourth case, we consider that $C_p(t)$ and $C_s(t)$ are (ii)–gH differentiable; that is, $C_p'(t)$ is given as in (2.7) and $C_s(t)$ is given by (2.5). Then we obtain the following system of ODE:

$$\begin{cases} \underline{C_p^{\alpha\prime}(t)} = k_{s\to p}\underline{C_{s_0}^{\alpha}}\mathrm{e}^{-k_{\mathrm{deg},s}t} + \lambda\overline{C_p^{\alpha}(t)}, \\ \overline{C_p^{\alpha\prime}(t)} = k_{s\to p}\overline{C_{s_0}^{\alpha}}\mathrm{e}^{-k_{\mathrm{deg},s}t} + \lambda\overline{C_p^{\alpha}(t)}, \\ \underline{C_p^{\alpha}(0)} = \underline{C_{p_0}^{\alpha}},\ \overline{C_p^{\alpha}(0)} = \overline{C_{p_0}^{\alpha}}, \\ \underline{C_s^{\alpha}(0)} = \underline{C_{s_0}^{\alpha}},\ \overline{C_s^{\alpha}(0)} = \overline{C_{s_0}^{\alpha}}, \end{cases} \quad \alpha \in [0,1]\,. \tag{2.11}$$

The solution of (2.1) (the (ii)–(ii)–gH solution) in terms of its α-levels is given by

$$\begin{cases} \underline{C_p^{\alpha}(t)} = C_1\mathrm{e}^{\lambda t} - \frac{k_{s\to p}\underline{C_{s_0}^{\alpha}}}{\lambda + k_{\mathrm{deg},s}}\mathrm{e}^{-k_{\mathrm{deg},s}t}, \\ \overline{C_p^{\alpha}(t)} = C_2\mathrm{e}^{\lambda t} - \frac{k_{s\to p}\overline{C_{s_0}^{\alpha}}}{k_{\mathrm{deg},s}+\lambda}\mathrm{e}^{-k_{\mathrm{deg},s}t}, \end{cases} \quad \alpha \in [0,1]\,,$$

where,

$$\begin{cases} C_1 = \underline{C_{p_0}^{\alpha}} + \frac{k_{s\to p}\underline{C_{s_0}^{\alpha}}}{\lambda + k_{\mathrm{deg},s}}, \\ C_2 = \overline{C_{p_0}^{\alpha}} + \frac{k_{s\to p}\overline{C_{s_0}^{\alpha}}}{k_{\mathrm{deg},s}+\lambda}, \end{cases} \quad \alpha \in [0,1]\,.$$

3. A first approach to the validation of the model

In Section 2, we obtained the solution of (2.1) in a general setting, that is, without consider specific values for the fuzzy initial data and parameters. In this section, we will validate the model considering some fuzzy initial data and estimating the unknown parameters via a combination of field data and a regression analysis for a specific chemical. As was said, one of the most used pesticides in pest control is the *thiamethoxam*, and therefore, we use some field data and reported information about this pesticide, in order to validate the model. For that, we collect some thiamethoxam concentration data in potato tubers harvested in a potato crop in a production field in Santander, Colombia. These data allow us to know the concentration of this chemical in the tubers at 3 different times. The samples used in laboratory were homogenized and extracted by the QuEChERS method [21] at the Chromatography and Mass Spectrometry laboratory of the Universidad Industrial de Santander (CROMASS). The results of the laboratory are shown in Table 1.

3.1. Initial data

Model (2.1) involves two initial data, namely C_{s_0} and C_{p_0}. We consider C_{s_0} as a fuzzification of the crisp value 45.3 μg kg^{-1}, which has been taken proportional to the value reported in [5] in its study of pesticide concentration in soil (see Tab. 4). In addition, we consider C_{p_0} as a fuzzification of the crisp value 16.39 μg kg^{-1}, which has been

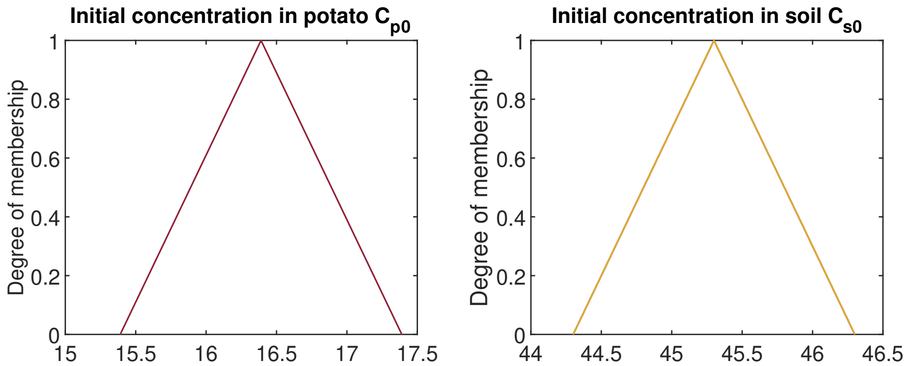

FIGURE 1. Fuzzy initial concentrations data C_{p_0} and C_{s_0}.

taken from the field data at $t = 0$ (see Tab. 1). Specifically, we consider the initial concentrations as triangular fuzzy numbers (for simplicity) with α-levels $[C_{s_0}]^\alpha = [\alpha + 44.3, 46.3 - \alpha]$ and $[C_{p_0}]^\alpha = [\alpha + 15.39, 17.39 - \alpha]$, for which $[C_{s_0}]^1 = \{45.3\}$ and $[C_{p_0}]^1 = \{16.39\}$ (see Fig. 1).

3.2. Parameters

Model (2.1) involves five parameters, namely, $k_{\text{growth},p}$, $k_{\text{deg},p}$, $k_{\text{deg},s}$, $k_{s\to p}$ and $k_{p\to s}$. We take $k_{\text{growth},p}$ as in [19], see Table 6. Thus, we must estimate $k_{\text{deg},p}$, $k_{\text{deg},s}$, $k_{s\to p}$ and $k_{p\to s}$. With respect to $k_{s\to p}$ and $k_{p\to s}$, according to [7], they are defined as

$$k_{s\to p} = \frac{23D_{\text{effe}}}{[r_p]^2 K_{sw}\rho_p}, \quad k_{p\to s} = \frac{23D_{\text{effe}}}{[r_p]^2 K_{pw}\rho_p},$$

where $D_{\text{effe}}(m^2 d^{-1})$ is the effective diffusivity of the pesticide in potato tissues; $r_p(m)$ is the radius of the potato tuber, $K_{sw}(\mathrm{L\,kg^{-1}})$ and $K_{pw}(\mathrm{L\,kg^{-1}})$ are the soil–water and potato–water partition coefficients of the pesticide, respectively, and $\rho_p(\mathrm{kg\,L^{-1}})$ is the potato density. These new parameters depend on particular soil and potato characteristics (water content in potato, lipid content in potato, carbohydrate content in potato, volumetric fraction of air in soil, volumetric fraction of organic matter in soil, and volumetric fraction of water in soil, among others); since we do not know this particular information on the soil and the potato, it is necessary to estimate them using other tools.

In order to estimate the unknown parameters, we use the data in Table 1; however, given the limited field data on thiamethoxam concentration in potato tubers, we need to obtain more data for a suitable estimation of parameters; thus, we use a local polynomial regression LOESS technique (see Sect. 3.2.2) on the data of Table 1 and the least squares theory, as described below.

3.2.1. Nonlinear least squares

The nonlinear least squares method [22] is a kind of least squares analysis used to fit a set of n observations with a model that is nonlinear in l unknown parameters ($n > l$). This method is used to estimate parameters of a nonlinear regression model by minimizing the squared residuals, the measured values or observed data, and the expected values. Consider a set of n observations, $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, and a curve (regression function) $y = f(x, \boldsymbol{\beta})$, which depends on the variable x as well as of l parameters $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_l)$, the aim is to find the vector $\boldsymbol{\beta}$ of parameters that minimizes the following sum squared residuals

$$SSR = \sum_{k=1}^{n} r_k^2 = \sum_{k=1}^{n} \left(y_k - f\left(x_k, \boldsymbol{\beta}\right)\right)^2.$$

We will use the SSR in two moments. First, it is used in the LOESS regression to estimate the intercept and scope in a linear regression on the field data in Table 1 considering a weight function, such that the fitted linear function is the best in the least squared sense. Second, it is used to estimate the unknown parameters in model (2.1) by minimizing the SSR, considering the data set obtained by LOESS and nonlinear regression functions. Below, we recall some preliminaries about LOESS.

3.2.2. Local polynomial regression (LOESS)

The local polynomial regression technique LOESS is a strategy to fit smooth curves to empirical data [23, 24]. Suppose that y_k, $k = 1, \ldots, n$, are observations of the dependent variable (the variable *concentration* in our case) and x_k the observations of the independent variable (the variable *time* in our case). Let $y_k = g(x_k) + \epsilon_k$, where $g(x)$ is a smooth function of x to be estimated, and ϵ_k are independent and identically distributed normal random variables with mean 0 and variance σ^2. Let x be a point at which we are going to compute an estimate $\hat{g}(x)$ of $g(x)$. It is necessary to define the proportion $\lambda \in [0, 1]$ of observations to be used for the local regression; the neighborhood size q for estimation in the local regression, which is given by λn truncated to an integer; the distance $d(x)$ of the qth-nearest x_k to x, and $w_k(x)$ a set of weights for the points (x_k, y_k) defined by

$$w_k(x) = W\left(\frac{|x_k - x|}{d(x)}\right), \text{ for } k = 1, \ldots, n,$$

where, $W(u)$ is a weight function for $u > 0$, such that $W(u) \geq 0$, with $W(u) = 0$ for $u > 1$, and non-increasing for $u \in (0, 1]$. To get $\hat{g}(x)$ (value of the fitted function at x), we fit a linear function on the independent variable to the dependent variable by weighted least squares with weight $w_k(x)$ in (x_k, y_k), as follows [25]:

$$l_k = \widehat{\beta}_{0w} + \widehat{\beta}_{1w} x_k,$$

where, $\widehat{\beta}_{1w} = \frac{\sum_{k=1}^{n} w_k (x_k - \bar{x}_w)(y_k - \bar{y}_w)}{\sum_{k=1}^{n} w_k (x_k - \bar{x}_w)^2}$ and $\widehat{\beta}_{0w} = \bar{y}_w - \widehat{\beta}_{1w} \bar{x}_{w_k}$, considering weighted means $\bar{x}_w = \frac{\sum_{k=1}^{n} w_k x_k}{\sum_{k=1}^{n} w_k}$ and $\bar{y}_w = \frac{\sum_{k=1}^{n} w_k y_k}{\sum_{k=1}^{n} w_k}$. Thus, the form of $\hat{g}(x)$ considering a linear estimation of y_k is given by (see [24]):

$$\hat{g}(x) = \sum_{k=1}^{n} l_k(x) y_k.$$

We apply the LOESS procedure for obtaining new data for the thiamethoxam concentration in potato tubers. We take the field data in Table 1, which means that $n = 3$; in addition, we assume $\lambda = 0.75$ which allows us use two data for each new estimation; it means that $q = 2$. We use RStudio to apply the LOESS regression by using the $loess(\cdot)$ function, which uses the tricube weight function $\left(W(u) = (1 - u^3)^3\right)$ to define the weight functions $w_k(x) = \left(1 - \left(\frac{|x_k - x|}{d(x)}\right)^3\right)^3$, where $|x_k - x| < d(x)$, for all x_k in the selected neighborhood of x. Table 2 collects the data obtained via LOESS.

Table 2. Input data from LOESS.

Time t_k (days)	Concentration y_k ($\mu\text{g}\,\text{kg}^{-1}$)
0	16.39
1	15.179259
2	12.930741
3	11.72
4	11.522245
5	11.012245
6	10.314848
7	9.555102
8	8.857755
9	8.347755
10	8.15

3.2.3. Parameter estimation

To estimate the degradation parameter of pesticide in potato tubers $k_{\text{deg},p}$ we use nonlinear least squares method (see Sect. 3.2.1). For that, we require to define a regression function $y = \widehat{C_p}(t, k_{\text{deg},p})$ on the data y_k from Table 2 such that $y_k = \widehat{C_p}(t_k, k_{\text{deg},p}) + \epsilon_k$, for $k = 1, ..., 11$. We consider the scenario for modeling pesticide concentration in potato tubers in which we assume an exponential decreasing behavior of the pesticide concentration in the tuber [5], as follows:

$$\begin{cases} \widehat{C_p}'(t) &= -k_{\text{deg},p}\widehat{C_p}(t), \\ \widehat{C_p}(0) &= 16.39, \end{cases} \tag{3.1}$$

where the value 16.39 has been taken from the field data in Table 2 at $t = 0$. Thus, we estimate $k_{\text{deg},p}$ such that it minimizes the gap (SSR) between the value observed (data in Tab. 2) and the value obtained by the regression function $\widehat{C_p}(t)$ given by model (3.1), that is,

$$\min_{k_{\text{deg},p}} \; SSR = \min_{k_{\text{deg},p}} \; \sum_{k=1}^{11} \left(y_k - \widehat{C_p}(t_k, k_{\text{deg},p})\right)^2 = \min_{k_{\text{deg},p}} \; \sum_{k=1}^{11} \left(y_k - 16.39\mathrm{e}^{-k_{\text{deg},p}t_k}\right)^2. \tag{3.2}$$

We use the Newton method to aproximate $\min\limits_{k_{\text{deg},p}} SSR$, for which the iterations are given by $k^{(s+1)}_{\text{deg},p} = k^{(s)}_{\text{deg},p} - \frac{SSR'\left(k^{(s)}_{\text{deg},p}\right)}{SSR''\left(k^{(s)}_{\text{deg},p}\right)}$, where

$$\frac{\partial SSR}{\partial k_{\text{deg},p}} = 32.78 \sum_{k=1}^{11} \left(y_k - 16.39\mathrm{e}^{-k_{\text{deg},p}t_k}\right) \cdot t_k \mathrm{e}^{-k_{\text{deg},p}t_k}, \text{ and}$$

$$\frac{\partial^2 SSR}{\partial k^2_{\text{deg},p}} = 32.78 \sum_{k=1}^{11} -y_k t_k^2 \mathrm{e}^{-k_{\text{deg},p}t_k} + 32.78 \left(-t_k^2 \mathrm{e}^{-2k_{\text{deg},p}t_k}\right).$$

Table 3. Result of minimization iterations. (3.2).

Iteration	SSR	Estimation	Convergence
0	360.7893	0	6.13
1	18.82518	0.05829214	2.02
2	3.532288	0.07713355	1.72×10^{-1}
3	3.428986	0.07890152	4.32×10^{-3}
4	3.428921	0.07894645	8.30×10^{-5}
5	3.428921	0.07894731	1.59×10^{-6}

Table 4. Thiamethoxam concentration in soil [5].

Time (days)	Concentration (μg kg^{-1})	
0	7582	45.3
1	4850	48.3542249
2	3700	36.8887902
3	3150	31.4053214
5	1450	14.4564178
7	420	4.1873762
14	30	0.2990983

By using the initial guess $k_{\mathrm{deg},p}^{(0)} = 0$, we carry out 5 iteration steps (see Tab. 3), where the final value is $k_{\mathrm{deg},p} = 0.078947$ in $SSR = 3.428921$.

On the other hand, to estimate $k_{\mathrm{deg},s}$ we need to obtain a thiamethoxam concentration in soil data set. Since we have no field data on thiamethoxam concentration in soil, we use soil pesticide concentration data proportional to those reported by [5] in its study on thiamethoxam concentration in soil (see Tab. 4). In this case, similarly to the case $k_{\mathrm{deg},p}$, we consider the regression function given by the crisp case solution of the model (2.3), and we estimate $k_{\mathrm{deg},s}$ such that it minimizes the squared residuals (SSR) between the observed values of the dataset and the values computed with the regression function to obtain the best fit of the regression function to the data in the least squares sense.

To estimate $k_{s\to p}$ and $k_{p\to s}$, we use the previously estimated parameters $k_{\mathrm{deg},p}$, $k_{\mathrm{deg},s}$, and we minimize the SSR (squared residuals) considering as regression function the solution for the potato pesticide concentration of the crisp case of the FIVP (2.1) on the data in Table 2, that is,

$$\begin{aligned}
\min_{(k_{s\to p},k_{p\to s})} SSR &= \min_{(k_{s\to p},k_{p\to s})} \sum_{k=1}^{11} r_k^2 \\
&= \min_{(k_{s\to p},k_{p\to s})} \sum_{k=1}^{11} \Bigg(y_k - \Bigg(\frac{k_{s\to p} C_{s_0}}{k_{p\to s} + k_{\mathrm{growth},p} + k_{\mathrm{deg},p} - k_{\mathrm{deg},s}} \left(\mathrm{e}^{-k_{\mathrm{deg},s} t_k} - \mathrm{e}^{-(k_{p\to s}+k_{\mathrm{growth},p}+k_{\mathrm{deg},p})t_k} \right) \\
&\qquad + C_{p_0} \mathrm{e}^{-(k_{p\to s}+k_{\mathrm{growth},p}+k_{\mathrm{deg},p})t_k} \Bigg) \Bigg)^2 \\
&= \min_{(k_{s\to p},k_{p\to s})} \sum_{k=1}^{11} \Bigg(y_k - \Bigg(\frac{45.3 k_{s\to p}}{k_{p\to s} + 0.030347} \left(\mathrm{e}^{-0.1876 t_k} - \mathrm{e}^{-(k_{p\to s}+0.217947)t_k} \right) + 16.39 \mathrm{e}^{-(k_{p\to s}+0.217947)t_k} \Bigg) \Bigg)^2 .
\end{aligned} \tag{3.3}$$

TABLE 5. Result of minimization iterations. (3.3).

Iteration	SSR	Estimation $k_{s\to p}$	Estimation $k_{p\to s}$	Convergence
0	694.4690	1	1	3.67
1	93.79722	0.4001766	0.552406	1.71
2	37.24385	0.0452268	–0.00757589	6.13
3	3.329989	–0.03626096	–0.2045454	1.36
4	1.170877	–0.03613011	–0.2110658	4.08×10^{-2}
5	1.168946	–0.03574021	–0.2100982	6.84×10^{-4}
6	1.168946	–0.03575724	–0.2101326	2.65×10^{-5}
7	1.168946	–0.03575658	–0.2101313	1.18×10^{-6}

TABLE 6. Parameters of the model (2.1) for thiamethoxam.

Parameter	Estimation
$k_{\deg,p}$	0.078947
$k_{\deg,s}$	0.1876
$k_{\text{growth},p}$	0.1390
$k_{s\to p}$	–0.03575658
$k_{p\to s}$	–0.2101313
$\lambda = -[k_{p\to s} + k_{\text{growth},p} + k_{\deg,p}]$	–0.0078157

In this case, we use the Gauss–Newton method to aproximate $\min\limits_{(k_{s\to p},k_{p\to s})} SSR$, for which the iterations are given by $\begin{pmatrix} k_{s\to p}^{(s+1)} \\ k_{p\to s}^{(s+1)} \end{pmatrix} = \begin{pmatrix} k_{s\to p}^{(s)} \\ k_{p\to s}^{(s)} \end{pmatrix} - (J_r^T J_r)^{-1} J_r^T r \left(k_{s\to p}^{(s)}, k_{p\to s}^{(s)}\right)$, where $r = [r_1, \ldots, r_{11}]^T$, and $J_r \in \mathbb{R}^{11,2}$ is the Jacobian matrix of r, given by $Jr = \begin{bmatrix} \frac{\partial r_k}{\partial k_{s\to p}} & \frac{\partial r_k}{\partial k_{p\to s}} \end{bmatrix}_{k=1,\ldots,11.}$ with

$$\frac{\partial r_k}{\partial k_{s\to p}} (k_{s\to p}, k_{p\to s}) = \frac{45.3}{k_{p\to s} + 0.030347} \left(\mathrm{e}^{-0.1876 t_k} - \mathrm{e}^{-(k_{p\to s}+0.217947)t_k}\right),$$

and

$$\begin{aligned} \frac{\partial r_k}{\partial k_{p\to s}} (k_{s\to p}, k_{p\to s}) = & \frac{-45.3 k_{s\to p}}{(k_{p\to s} + 0.030347)^2} \left(\mathrm{e}^{-0.1876 t_k} - \mathrm{e}^{-(k_{p\to s}+0.217947)t_k}\right) \\ & + \left(\frac{45.3 k_{s\to p}}{k_{p\to s} + 0.030347} - 16.39\right) t_k \mathrm{e}^{-(k_{p\to s}+0.217947)t_k}. \end{aligned}$$

By using the initial guesses $k_{p\to s} = 1$ and $k_{s\to p} = 1$, we carry out 7 iteration steps (see Tab. 5), where the final values are $k_{p\to s} = -0.2101313$ and $k_{s\to p} = -0.03575658$ in $SSR = 1.168946$.

In the estimation process of $k_{\deg,p}$, $k_{\deg,s}$, $k_{s\to p}$ and $k_{p\to s}$, we use the function $nls(\cdot)$ of RStudio. Table 6 collects the estimation of the parameters involved in the system (2.1).

Remark 3.1. In previous analysis the parameters $k_{\text{growth},p}$, $k_{\deg,p}$, $k_{\deg,s}$, $k_{s\to p}$ and $k_{p\to s}$ has been considered as real numbers; however, given the nondeterministic nature of these parameters they could be considered as fuzzy numbers, which imply a new analysis of the fuzzy initial value problem (2.1).

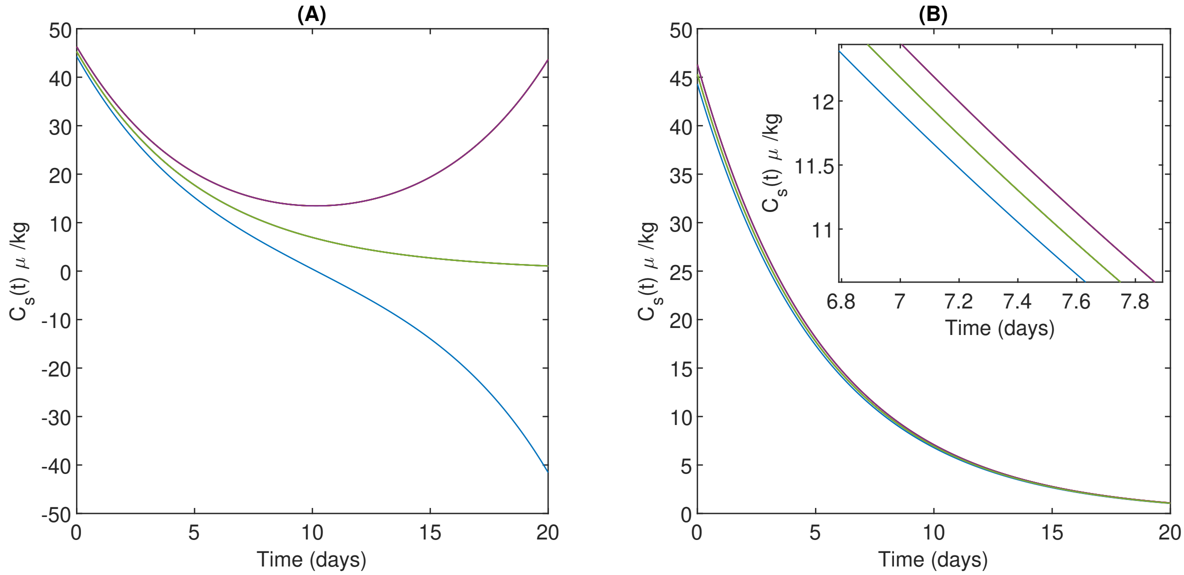

FIGURE 2. Pesticide concentration in soil over time. (A): Evolution of $C_s(t)$ in the case where $C_s(t)$ is (i)–gH differentiable. (B): Evolution of $C_s(t)$ in the case where $C_s(t)$ is (ii)–gH differentiable.

3.3. Computing the solution of (2.1)

We solve the fuzzy ordinary differential system (2.1) for the thiamethoxam, considering the initial data as in Section 3.1 and the estimated parameters shown in Table 6. First we solve the system for $C_s(t)$. Figure 2 shows the (i)–gH solution and the (ii)–gH solution of (2.3). In both cases, the 1-levels (green curves) of the (i) and (ii)–gH solutions correspond to the crisp case, while the support is determined by the blue and purple curves. We observe that the (ii)–gH solution for $C_s(t)$ has a decreasing exponential fuzzy behavior as expected, and its support length decreases, as time increases, while the support length of the (i)–gH solution increases, as time increases. In the case of (i)–gH solution, even the curve that defines its 1-level is positive and converges to zero asymptotically, the lower function that describes the support of the (i)–gH solution (blue curve) reaches negative values, which has not physical sense. Now, knowing $C_s(t)$ we solve the differential equation for $C_p(t)$. The solution $C_p(t)$ involves four cases according the analysis discussed in Section 2.2, because we have two types of derivatives for both $C_s(t)$ and $C_p(t)$, and we find $C_p(t)$ after replacing $C_s(t)$ in the differential equation of $C_p(t)$. This generates four possible solutions, which are shown in Figure 3, namely, the (i)-(i), (i)-(ii), (ii)-(i) and (ii)–(ii)–gH solutions. The (i)–(ii)–gH solution and the (ii)–(ii)–gH solution of (2.1) show a fuzzy exponential decreasing behavior as expected. The (i)–(i)–gH solution shows an increase in the support of its solution, even the curve that defines its 1-level is an exponential type one (see Fig. 3A, green curve). Even more, the solution reaches negative values for large times, which is not of physical interest. The increase in the support of the solution $C_p(t)$ is due to the corresponding increase of the support of $C_s(t)$ as shown in Figure 2(A). The (ii)–(i)–gH solution has not a monotonic behavior in its support; it has a critical point at $t = t_1 = \frac{\ln(k-\lambda-k_{s\to p}) - \ln(-k_{s\to p})}{k-\lambda} \approx 9.55106946$, where $C_p(t_1)$ is a singleton. For $t > t_1$ it is not difficult to verify that the α-levels $[C_p(t)]^\alpha = [\underline{C_p(t)}, \overline{C_p(t)}]$ of the (ii)–(i)–gH solution $C_p(t)$ do not define a fuzzy number; however, the family of α-levels given by $[\overline{C_p(t)}, \underline{C_p(t)}]$ defines a fuzzy function that is not (ii)–gH differentiable but it is (i)–gH differentiable.

In this sense, the cases that present a physical interpretation of the behavior of $C_p(t)$ are given by the cases (i)-(ii) (see Sect. 2.2.2) and (ii)–(ii) (see Sect. 2.2.4).

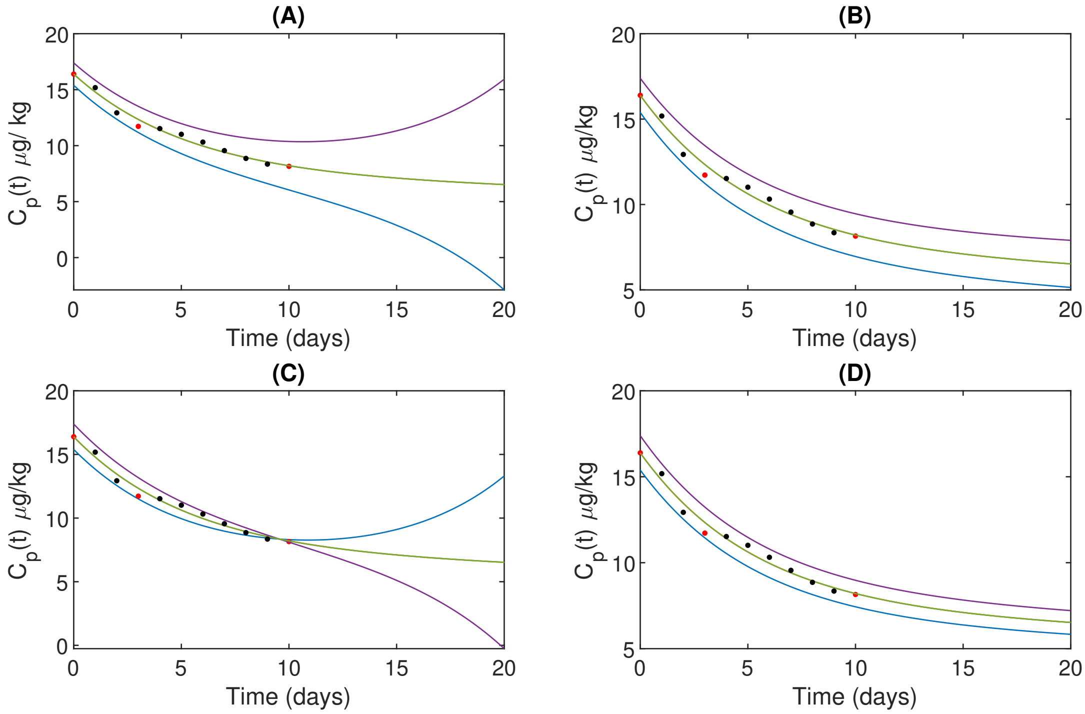

FIGURE 3. Pesticide concentration in potato over time. (A) Evolution of $C_p(t)$ in the case where $C_p(t)$ and $C_s(t)$ are (i)–gH differentiable. (B) Evolution of $C_p(t)$ in the case where $C_p(t)$ is (i)–gH differentiable and $C_s(t)$ is (ii)–gH differentiable. (C) Evolution of $C_p(t)$ in the case where $C_p(t)$ is (ii)–gH differentiable and $C_s(t)$ is (i)–gH differentiable. (D) Evolution of $C_p(t)$ in the case where $C_p(t)$ and $C_s(t)$ are (ii)–gH differentiable. In the four cases, each figure shows the support ($\alpha = 0$; blue and purple lines) and height ($\alpha = 1$; green line) functions of the corresponding solution $C_p(t)$, the dots in red color are the field data while the blank ones are the data in Table 2.

4. A second approach. A Takagi–Sugeno–Kang model (TSK)

To establish an alternative modeling approach for determining the degradation of the thiamethoxam concentration in potato tubers, we propose using a Takagi–Sugeno–Kang type fuzzy rule-based model to approximate the variation $\Delta C_p(t)$. This type of model emulates the human reasoning process based on fuzzy inference rules [20] and it is applied in several applied areas. For instance, the decision making theory [26, 27], neural network training [28], control systems design [29–31], risk analysis [32], and estimation of parameters [33, 34], among others. The start point is the functional relationship between the input and output variables according to a set of the inference rules, which can be formulated as follows:

$$\text{If } x_1 \text{ is } A_{j1}, x_2 \text{ is } A_{j2}, \ldots, \text{ and } x_m \text{ is } A_{jm}, \text{ then } Y_j = f_j(x_1, x_2, \ldots, x_m),$$

where $x_1, x_2, \ldots, x_m$ are the input variables in the universes $X_1, X_2, \ldots, X_m$ respectively, with values in fuzzy sets $A_{j1}, \ldots, A_{jm}$, $j = 1, 2, \ldots, N$ and Y_i is the consequent function, where N represents the number of fuzzy rules. One considers a t-norm operator "i" of the fuzzy sets and then, the output value w_j for each rule j by $w_j = i(A_{j1}(x_1), A_{j2}(x_2), \ldots, A_{jm}(x_m))$ is computed. Finally, one obtains the final value "y" of the model through the expression $y = \frac{\sum_{(j=1)}^{N}(w_j Y_j)}{\sum_{(j=1)}^{N} w_j}$ [20].

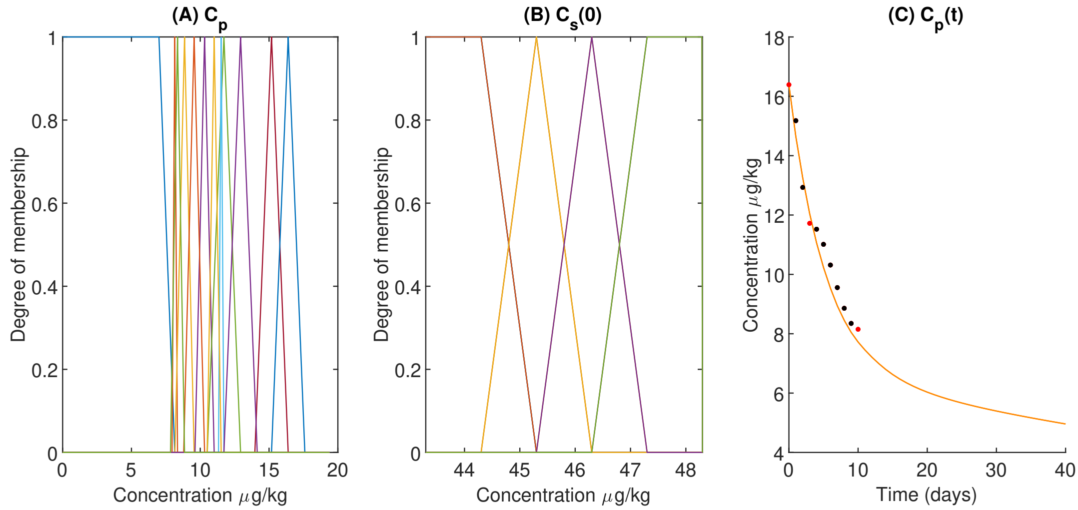

FIGURE 4. Input variables in the TSK model. (A) Linguistic variable concentration of pesticide in potato. (B) Linguistic variable initial concentration of pesticide in soil. (C) The orange curve is the solution $C_p(t)$ obtained through the designed TSK model; the dots in red color are the field data while the blank ones are the data in Table 2.

Thus, as an alternative for modeling the evolution of the thiamethoxam concentration in potato $C_p(t)$, we design a TSK model that allows us to describe the variation $\Delta C_p(t)$. The general idea is to use the discrete version of the differential system (2.1) creating a sequence of values that approximate the solution $C_p(t)$. For that, we take the pesticide concentration in potato C_p and the initial pesticide concentration in soil $C_s(0) = C_{s_0}$ as the input linguistic variables. Then, we define the linguistic terms of the variable C_p considering the provided data by Table 2 and represent them as triangular and trapezoidal fuzzy numbers (see Fig. 4) as follows:

$$
\begin{array}{ll}
C_{p_0} = \langle 15.1793, 16.39, 17.6007\rangle, & C_{p_1} = \langle 13.9685, 15.1793, 16.39\rangle, \\
C_{p_2} = \langle 10.6822, 12.9307, 15.1793\rangle, & C_{p_3} = \langle 10.5093, 11.72, 12.9307\rangle, \\
C_{p_4} = \langle 11.3245, 11.5223, 11.72\rangle, & C_{p_5} = \langle 10.5022, 11.0123, 11.5223\rangle, \\
C_{p_6} = \langle 9.6176, 10.3149, 11.0123\rangle, & C_{p_7} = \langle 8.7954, 9.5551, 10.3149\rangle, \\
C_{p_8} = \langle 8.1604, 8.8578, 9.5551\rangle, & C_{p_9} = \langle 7.8378, 8.3478, 8.8578\rangle, \\
C_{p_{10}} = \langle 7.9522, 8.15, 8.3478\rangle, & C_{p_{11}} = \langle 0, 0, 7.9523, 8.15\rangle.
\end{array}
$$

In addition, we define the linguistic terms of the variable C_{s_0} by the following triangular and trapezoidal fuzzy numbers (see Fig. 4):

$$
\begin{array}{ll}
C_{s_l} = \langle 42.3, 43.3, 44.3, 45.3\rangle, & C_{s_{ml}} = \langle 44.3, 45.3, 46.3\rangle, \\
C_{s_{mh}} = \langle 45.3, 46.3, 47.3\rangle, & C_{s_h} = \langle 46.3, 47.3, 48.3, 49.3\rangle.
\end{array}
$$

To define the inference rules, we consider all possible combinations of the linguistic terms of C_p with the linguistic terms of C_{s_0}. Here, we define 48 inference rules whose antecedent parts are presented in Table 7, as well as we define the consequent function $\Delta C_p(t)$ for each inference rule number j, for $j = 1, \ldots, 48$ as follows:

$$
\Delta_j C_p(t) = k_{s\to p}\mu_{j_{C_{s_0}}}(C_{s_0})C_{s_0}\mathrm{e}^{-k_{\mathrm{deg},s}t} + \lambda\mu_{j_{C_p}}(C_p(t))C_p(t)
$$

TABLE 7. Antecedent of inference rules.

n°	Rule	n°	Rule
1	If C_p is C_{p_0} and C_{s_0} is C_{s_l}	25	If C_p is C_{p_0} and C_{s_0} is $C_{s_{mh}}$
2	If C_p is C_{p_1} and C_{s_0} is C_{s_l}	26	If C_p is C_{p_1} and C_{s_0} is $C_{s_{mh}}$
3	If C_p is C_{p_2} and C_{s_0} is C_{s_l}	27	If C_p is C_{p_2} and C_{s_0} is $C_{s_{mh}}$
4	If C_p is C_{p_3} and C_{s_0} is C_{s_l}	28	If C_p is C_{p_3} and C_{s_0} is $C_{s_{mh}}$
5	If C_p is C_{p_4} and C_{s_0} is C_{s_l}	29	If C_p is C_{p_4} and C_{s_0} is $C_{s_{mh}}$
6	If C_p is C_{p_5} and C_{s_0} is C_{s_l}	30	If C_p is C_{p_5} and C_{s_0} is $C_{s_{mh}}$
7	If C_p is C_{p_6} and C_{s_0} is C_{s_l}	31	If C_p is C_{p_6} and C_{s_0} is $C_{s_{mh}}$
8	If C_p is C_{p_7} and C_{s_0} is C_{s_l}	32	If C_p is C_{p_7} and C_{s_0} is $C_{s_{mh}}$
9	If C_p is C_{p_8} and C_{s_0} is C_{s_l}	33	If C_p is C_{p_8} and C_{s_0} is $C_{s_{mh}}$
10	If C_p is C_{p_9} and C_{s_0} is C_{s_l}	34	If C_p is C_{p_9} and C_{s_0} is $C_{s_{mh}}$
11	If C_p is $C_{p_{10}}$ and C_{s_0} is C_{s_l}	35	If C_p is $C_{p_{10}}$ and C_{s_0} is $C_{s_{mh}}$
12	If C_p is $C_{p_{11}}$ and C_{s_0} is C_{s_l}	36	If C_p is $C_{p_{11}}$ and C_{s_0} is $C_{s_{mh}}$
13	If C_p is C_{p_0} and C_{s_0} is $C_{s_{ml}}$	37	If C_p is C_{p_0} and C_{s_0} is C_{s_h}
14	If C_p is C_{p_1} and C_{s_0} is $C_{s_{ml}}$	38	If C_p is C_{p_1} and C_{s_0} is C_{s_h}
15	If C_p is C_{p_2} and C_{s_0} is $C_{s_{ml}}$	39	If C_p is C_{p_2} and C_{s_0} is C_{s_h}
16	If C_p is C_{p_3} and C_{s_0} is $C_{s_{ml}}$	40	If C_p is C_{p_3} and C_{s_0} is C_{s_h}
17	If C_p is C_{p_4} and C_{s_0} is $C_{s_{ml}}$	41	If C_p is C_{p_4} and C_{s_0} is C_{s_h}
18	If C_p is C_{p_5} and C_{s_0} is $C_{s_{ml}}$	42	If C_p is C_{p_5} and C_{s_0} is C_{s_h}
19	If C_p is C_{p_6} and C_{s_0} is $C_{s_{ml}}$	43	If C_p is C_{p_6} and C_{s_0} is C_{s_h}
20	If C_p is C_{p_7} and C_{s_0} is $C_{s_{ml}}$	44	If C_p is C_{p_7} and C_{s_0} is C_{s_h}
21	If C_p is C_{p_8} and C_{s_0} is $C_{s_{ml}}$	45	If C_p is C_{p_8} and C_{s_0} is C_{s_h}
22	If C_p is C_{p_9} and C_{s_0} is $C_{s_{ml}}$	46	If C_p is C_{p_9} and C_{s_0} is C_{s_h}
23	If C_p is $C_{p_{10}}$ and C_{s_0} is $C_{s_{ml}}$	47	If C_p is $C_{p_{10}}$ and C_{s_0} is C_{s_h}
24	If C_p is $C_{p_{11}}$ and C_{s_0} is $C_{s_{ml}}$	48	If C_p is $C_{p_{11}}$ and C_{s_0} is C_{s_h}

where, $\mu_{j_{C_{s_0}}}(C_{s_0})$ and $\mu_{j_{C_p}}(C_p(t))$ represent the degree of membership of C_{s_0} and $C_p(t)$ to the linguistic terms set in the variable C_{s_0} and C_p respectively involved in each rule j according to Table 7.

Following the inference process in Section 4 the variation $\Delta C_p(t)$ is computed as

$$\Delta C_p(t) = \frac{\sum_{(j=1)}^{40}(w_j \Delta_j C_p(t))}{\sum_{(j=1)}^{40} w_j}, \tag{4.1}$$

where, $w_j = i(\mu_{j_{C_{s_0}}}(C_{s_0}), \mu_{j_{C_p}} C_p(t)) = \min\{\mu_{j_{C_{s_0}}}(C_{s_0}), \mu_{j_{C_p}}(C_p(t))\}$. We use the estimated $\Delta C_p(t)$ by the designed TSK model in (4.1) to approximate $C_p(t)$ by $C_p(t+1) = C_p(t) + \Delta C_p(t)$, from which we obtain the curve showed in Figure 4.

5. Comparison of the two approaches

Figure 5 shows the comparison between $C_p(t)$ modeled by fuzzy ordinary differential equations (see Sect. 2, more specifically the cases in Sects. 2.2.2 and 2.2.4), and the $C_p(t)$ modeled using a fuzzy logic model (TSK model; see Sect. 4). We can observe that the $C_p(t)$ obtained by the fuzzy logic approach (TSK model, see Fig. 4) fits within the solution support of the two cases with physical interpretation in the fuzzy differential equations model, describing a similar and consistent behavior of $C_p(t)$ in both approaches.

6. Conclusions

We used fuzzy modeling tools to describe the behavior of pesticide concentration in potato tubers. We proposed and solved a fuzzy initial value problem to model the pesticide concentration over time in potato

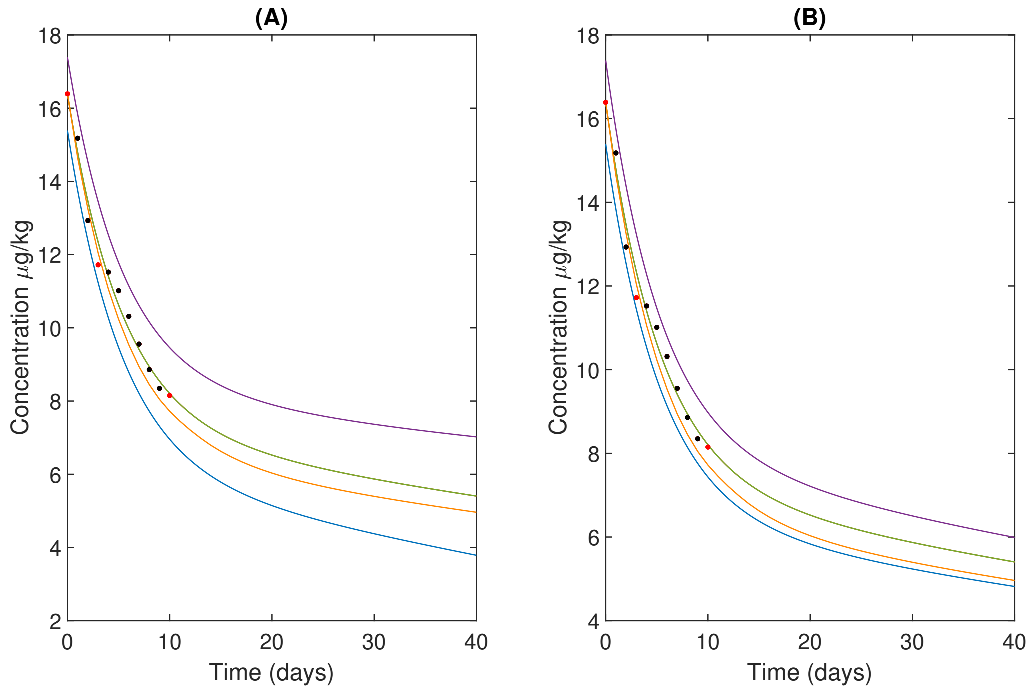

FIGURE 5. First approach vs second approach. (A): Evolution of $C_p(t)$ in the case where $C_p(t)$ is (i)–gH differentiable and $C_s(t)$ is (ii)–gH differentiable. (B): Evolution of $C_p(t)$ in the case where $C_p(t)$ and $C_s(t)$ are (ii)–gH differentiable. Each figure shows the support ($\alpha = 0$; blue and purple lines) and the height ($\alpha = 1$; green line) functions of the solution in the cases (i)–(ii)–gH and (ii)–(ii)–gH derivative with the curve of $C_p(t)$ based on the designed TSK model (orange curve); the dots in red color are the field data while the blank ones are the data in Table 2.

tubers. We validated the fuzzy differential equation model by analyzing the residual of thiamethoxam in a potato crop in Santander, Colombia, for which we obtained new data and estimated the degradation parameters in potato and soil, and the diffusion parameters between potato and soil using statistical estimation tools. In a second approach, we used fuzzy logic to model the time variation of $C_p(t)$ by designing a TSK model that allowed us to describe $C_p(t)$. Both approaches model the behavior of thiamethoxam concentration over time from field data. The advantage of our mathematical models is that they reveal good behavior despite the very reduced amount of (fuzzy) data. Our results could be applied to the study of residual behavior of a large class of pesticides in potato crops, and the mathematical analysis could also be explored in other dynamical systems.

Acknowledgements

The first author was supported by Minciencias-Colombia, project entitled "Formación de Capital Humano de Alto Nivel para el Departamento de Santander en la Universidad Industrial de Santander", code BPIN 2020000100536. The second author has been supported by Vicerrectoría de Investigación y Extensión of the Universidad Industrial de Santander.

References

[1] FAO/ESS, Production/crops and livestock products. Metadata [dataset] (2023). https://www.fao.org/faostat/en/#data/QCL/metadata.

[2] F. Saeed, S.D. Dangol, M.H. Hashmi, Md.J. Hossain and A. Bakhsh, Role of genetic engineering in improving potato production, in Potato Production Worldwide, Elsevier (2023) 303–315.

[3] P. Maienfisch, M. Angst, F. Brandl, W. Fischer, D. Hofer, H. Kayser, W. Kobel, A. Rindlisbacher, R. Senn, A. Steinemann and H. Widmer, Chemistry and biology of thiamethoxam: a second generation neonicotinoid. *Pest Manage. Sci.* **57** (2001) 906–913.

[4] L.M. He, J. Troiano, A. Wang and K. Goh, Environmental chemistry, ecotoxicity, and fate of lambda-cyhalothrin, in Reviews of Environmental Contamination and Toxicology. Reviews of Environmental Contamination and Toxicology. Vol. 195, edited by D.M. Whitacre. Springer, New York, NY (2008). https://doi.org/10.1007/978-0-387-77030-7_3.

[5] S.H. Abd-Alrahman, Residue and dissipation kinetics of thiamethoxam in a vegetable-field ecosystem using QuEChERS methodology combined with HPLC–DAD. *Food Chem.* **159** (2014) 1–4.

[6] X. Xiao, Y. Gong, Z. Li and P. Fantke, Improving pesticide uptake modeling into potatoes: considering tuber growth dynamics. *J. Agric. Food Chem.* **69** (2021) 3607–3616.

[7] Z. Li and P. Fantke, Considering degradation kinetics of pesticides in plant uptake models: proof of concept for potato. *Pest Manage. Sci.* **79** (2023) 1154–1163.

[8] R. Juraske, C.S. Mosquera-Vivas, A. Erazo-Velásquez, G. García-Santos, M.B. Berdugo-Moreno, J. Diaz-Gomez, *et al.*, Pesticide uptake in potatoes: model and field experiments. *Environ. Sci. Technol.* **45** (2011) 651–657.

[9] P. Fantke, R. Charles, L.F. de Alencastro, R. Friedrich and O. Jolliet, Plant uptake of pesticides and human health: dynamic modeling of residues in wheat and ingestion intake. *Chemosphere* **85** (2011) 1639–1647.

[10] B. Bede, I.J. Rudas and A.L. Bencsik, First order linear fuzzy differential equations under generalized differentiability. *Inform. Sci.* **177** (2007) 1648–1662.

[11] B. Bede and L. Stefanini, Generalized differentiability of fuzzy-valued functions. *Fuzzy Sets Syst.* **230** (2013) 119–141.

[12] Y. Chalco-Cano, A. Rufián-Lizana, H. Román-Flores and M.D. Jiménez-Gamero, Calculus for interval-valued functions using generalized Hukuhara derivative and applications. *Fuzzy Sets Syst.* **219** (2013) 49–67.

[13] E.J. Villamizar-Roa, V. Angulo-Castillo and Y. Chalco-Cano, Existence of solutions to fuzzy differential equations with generalized Hukuhara derivative via contractive like mapping principles. *Fuzzy Sets Syst.* **265** (2015) 24–38.

[14] V. Angulo-Castillo, Y. Chalco-Cano, A. Khastan and E.J. Villamizar-Roa, Applications of generalized fixed points theorems to the existence of uncertain differential equations with finite delay. *J. Iran. J. Fuzzy Syst.* **205** (2020) 1–15.

[15] A. Khastan and R. Rodríguez-López, On the solutions to first order linear fuzzy differential equations. *Fuzzy Sets Syst.* **295** (2016) 114–135.

[16] V. Angulo-Castillo, Y. Chalco-Cano, A. Khastan and É.J. Villamizar-Roa, Applications of generalized fixed points theorems to the existence of uncertain differential equations with finite delay. *Iran. J. Fuzzy Syst.* **17** (2020) 1–15.

[17] R. Osuna-Gómez, T.M. da Costa, Y. Chalco-Cano and B. Hernández-Jiménez, Quasilinear approximation for interval-valued functions via generalized Hukuhara differentiability. *Computat. Appl. Math.* **41** (2022) Paper No. 149.

[18] R. Osuna-Gómez, T.M. da Costa, B. Hernández-Jiménez and G. Ruiz-Garzón, Necessary and sufficient conditions for interval-valued differentiability. *Math. Meth. Appl. Sci.* **46** (2023) 2319–2333.

[19] S. Trapp, A. Cammarano, E. Capri, F. Reichenberg and P. Mayer, Diffusion of PAH in potato and carrot slices and application for a potato model. *Environ. Sci. Technol.* **41** (2007) 3103–3108.

[20] E. Massad, N.R.S. Ortega, L.C. de Barros and C.J. Struchiner, Fuzzy Logic in Action: Applications in Epidemiology and Beyond. Vol. 232. Springer Science & Business Media (2009).

[21] A. Wilkowska and M. Biziuk, Determination of pesticide residues in food matrices using the QuEChERS methodology. *Food Chem.* **125** (2011) 803–812.

[22] D.M. Bates and J.M. Chambers, Nonlinear models, in Chapter 10 of Statistical Models in S, edited by J.M. Chambers and T.J. Hastie. Wadsworth & Brooks/Cole (1992).

[23] W.S. Cleveland, S.J. Devlin and E. Grosse, Regression by local fitting: methods, properties, and computational algorithms. *J. Econom.* **37** (1988) 87–114.

[24] W.S. Cleveland, E. Grosse and W.M. Shyu, Local regression models, in Chapter 8 of Statistical Models in S, edited by J.M. Chambers and T.J. Hastie. Wadsworth & Brooks/Cole (1992).

[25] Y. Dodge, Weighted least-squares method, in The Concise Encyclopedia of Statistics. Springer, New York, NY (2008).

[26] P.S. Duarte, L.E. Mastrocolla, P.S. Farsky, C.R.E.P.S. Sampaio, P.A. Tonelli, L.C. Barros, N.R. Ortega and J.C.R. Pereira, Selection of patients for myocardial perfusion scintigraphy based on fuzzy sets theory applied to clinical-epidemiological data and treadmill test results. *Braz. J. Med. Biol. Res.* **39** (2006) 9–18.

[27] A. Ramathilagam and P. Pitchipoo, Modeling and development of fuzzy logic-based intelligent decision support system. *Roman. J. Inform. Sci. Technol.* **25** (2022) 58–79.

[28] A. Dimitriadis, J. Theocharis and G. Vachtsevanos, Front: a novel method for training fuzzy neural networks with TSK rules. *Control Intell. Syst.* **26** (1998) 92–101.

[29] N.M. Ghasem, Design of a fuzzy logic controller for regulating the temperature in industrial polyethylene fluidized bed reactor. *Chem. Eng. Res. Des.* **84** (2006) 97–106.

[30] S. Yordanova, TSK model-based fuzzy logic control of carbon dioxide concentration in rooms. *Mechatronic Syst. Control* **46** (2018) 32–38.

[31] A.I. Szedlak-Stinean, R.E. Precup, E.M. Petriu, R.C. Roman, E.L. Hedrea and C.A. Bojan-Dragos, Extended Kalman filter and Takagi–Sugeno fuzzy observer for a strip winding system. *Expert Syst. Appl.* **208** (2022) Paper No. 118215.

[32] G.P. Silveira and L.C. de Barros, Analysis of the dengue risk by means of a Takagi–Sugeno–style model. *Fuzzy Sets Syst.* **277** (2015) 122–137.

[33] N.R.S. Ortega, P.C. Sallum and E. Massad, Fuzzy dynamical systems in epidemic modeling. *Kybernetes* **29** (2000) 201–218.

[34] E.J. Villamizar-Roa, L.V. Espitia-Cruz and G. Arenas-Díaz, Intrinsic growth rate and evolution of the Premnotrypes Vorax population using fuzzy information. *Biosystems* **237** (2024) Paper No. 105161.