Modelling pesticide uptake by potatoes through an ordinary differential equation coupled with a dispersion-advection equation

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1 Introduction

Potato plants are cultivated in more than one hundred countries across different continents because of their extraordinary ability to adapt to different weather and soil conditions, surpassed only by wheat, rice and corn, being consumed by more than one billion people. With a global production of 324 million tons in 2010, potato is the fourth most important food crop (or fifth if we consider sugar cane, a plant that is not always consumed as food) and it is one of the most important vegetables consumed worldwide [1]. Potato plants' agronomic efficiency guarantees the use of several types of soils destined to food production, which contributes to increase the total potato cropping area in a global scenario of fast population growth and economic development. All over the world, the main limiting factor to potato cropping is the plant's susceptibility to a great number of pests and diseases, some of them capable of causing serious damage to potato production. This obliges the use of many and varied types of pesticides that may cause serious environmental and alimentary problems [2-4].

Even when taking into account that the most recent agronomic management techniques, suggested by the integrated production systems, reduce risks of environment and food contamination it is very important that managers, technicians and researchers learn how to estimate the cumulative potential of pesticides in potatoes, which will enable them to recommend new products and technologies in order to have economically and environmentally sustainable productions. The United Nations Food and Agriculture Organization is currently promoting the tuber as an efficient food crop (potatoes are low-fat, high-carbohydrate food) that can improve food security in developing countries. Approximately 80% of the potato plant can be used for human consumption, a significantly higher percentage than that of cereals like corn and wheat.

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Several studies indicate the presence of pesticides and organic substances in potatoes [5-15] but none of them present a theoretically acceptable model that one can use to estimate pesticide concentrations in potato and in soil solution by the ordinary differential equation (ODE) coupled with a dispersion-advection equation (DAE) system. Three potato-specific plant uptake models were recently published [13,14,16], using Fick's second law for modelling the diffusive flow of a pesticide through potato tissues. These three models enable the estimation of pesticide bioconcentration factors in potato tubers, by using a known concentration of pesticide in soil. Trapp and co-workers [16] suggest that the transfer of pesticide mass occurs through the potato tissues, predominantly by the soil solution. This model makes it possible to estimate the diffusivity of organic substances in soil for potatoes, and helps significantly to elaborate useful mathematical models to determine the potato's concentration of non-ionic organic pesticides in the soil solution. Paraíba and Kataguiri [13], based on the work of Trapp and co-workers [16], presented a model that estimates the bioconcentration factor (BCF) of pesticides in potatoes supposing that the pesticide in the soil solution is absorbed by the potato by passive diffusion, following Fick's second law and the pesticides' degrade in the soil according to a first-order kinetic equation. Juraske and co-workers [14] also presented and evaluated a dynamic model of first-order kinetic equation for uptake of pesticides in potatoes, with measurements performed in a field trial in the region of Boyacá, Colombia.

It is extremely difficult to assess pesticides' environmental fate, as some of these substances are quite mobile that can take different pathways before they are effectively removed from the soil system. From the water and potato contamination point of view, soil plays a central role in pesticides uptake and transport. Soil is the main geologic compartment where degradation can occur and pesticides are likely to be attenuated before they leach to groundwater or uptake to potato. The soil capability to adsorb (sorption + adsorption) pesticides is affected by the occurrence of organic matter and soil mineral constituents, and soil ionic charge. Additionally, pesticides potential to leach to groundwater is affected by soil permeability, soil texture, water table fluctuations, and water content. Pavlis and co-workers [17] present a cross-analysis of different models of pesticide fate and the environmental indicators to underscore their relative strengths, weaknesses, similarities and dissimilarities.

The objective of this work is to present a model that simulates pesticide uptake by potatoes using a system with two differential equations, where one equation describes pesticide uptake by potatoes and the other one describes the pesticide lixiviation in soil. It was assumed that uptake and lixiviation occur, respectively, by diffusion of the pesticide through potato tissues and by diffusion and advection of the pesticide in soil profile. Uptake was described by an ordinary differential equation (ODE) that was coupled to a dispersion-advection equation (DAE). These equations describe the kinetics of the pesticide in potatoes and in soil profile, respectively. The coupled equations (ODE-DAE) were numerically solved through a finite difference method, programmed in Matlab® system, and used to simulate uptake of pesticides by potatoes.

2 Materials and methods

2.1 Mathematical modelling of pesticide uptake by potatoes, using an ODE coupled with a DAE

2.1.1 Model development

The pesticides' uptake by potato from the soil solution, by passive diffusion, and the dilution by growth and enzymatic metabolism of pesticide in potato were modelled by

$$\frac{dC_p}{dt} = k_u C_w(\delta_r, t) - k_p C_p \qquad (1)$$

where C_p (mg kg^{-1}) is the pesticide concentration in the potato, $C_w = C_w(\delta_r, t)$ (mg L^{-1}) is the pesticide concentration in soil solution in a day t (day), δ_r (m) is the average depth of a potato inside the soil, k_p (day^{-1}) is the dilution and metabolism rate, and k_u (L kg^{-1} day^{-1}) is the rate of pesticide uptake by the potato. The initial concentration of pesticide in potatoes is assumed to be null, that is, $C_p(0) = 0$.

The pesticide uptake rate of soil solution was estimated supposing a passive diffusion through potato tissues with the diffusion coefficient as in [16], given by $k_u = \frac{23 D_p}{(r_p)^2 \rho_p k_{sw}}$, where D_p (m^{2}day^{-1}) is the effective diffusion coefficient of pesticide through potato tissues, r_p (m) is the average radius of the potato, ρ_p (kg L^{-1}) is the density of the potato, and k_{sw} (dimensionless) is the soil-water partition coefficient of the pesticide. Potato density is necessary to define correctly the pesticide uptake rate with a measured unit of L kg^{-1}day^{-1}, while the pesticide uptake rate is inversely proportional to potato density, see [18].

The dimensionless soil-water partition coefficient of the pesticide was calculated by $k_{sw} = \rho_s f_{oc} k_{oc} + f_w + f_a k_{aw}$, where ρ_s (L kg^{-1}) is the total soil density. The f_{oc}, f_w and f_a coefficients are the volumetric fractions of organic carbon, water and air of the soil, respectively. The parameter k_{oc} $(\mathrm{L\ kg^{-1}})$ is the pesticide organic carbon-water partition coefficient and it was estimated by the expression given by $k_{oc} = 10^{(0.1+0.81\log k_{ow})}$, see [19,20], where k_{ow} is the pesticide's octanol-water partition coefficient and k_{aw} (dimensionless) is the pesticide's air-water partition coefficient that is estimated by $k_{aw} = \dfrac{P_v P_m}{S_w R_g (273+T)}$, where $(T = 25^{\circ}\mathrm{C})$ is the air temperature, $(R_g = 8.314\mathrm{Pa\ m^3 mol^{-1}})$ is the universal gas constant, P_v (Pa) is the pesticide's vapour pressure, P_m $(\mathrm{g\ mol^{-1}})$ is its molar mass and S_w $(\mathrm{g\ m^{-3}})$ is its water solubility.

The pesticide's coefficient of effective diffusion through potato tissues was estimated by $D_p = p_w \tau_w D_w$, where τ_w (dimensionless) is a coefficient of soil tortuosity and p_w (dimensionless) is the volumetric fraction of pesticide dissolved in the water phase of potato tissue, calculated by $p_w = w_p / k_{pw}$, in which w_p is the pore water fraction in the potato tissue, k_{pw} (dimensionless) is the potato-water partition coefficient of the pesticide, estimated by the equation $k_{pw} = w_p + f_{chp} k_{chw} + 0.82 L_p (k_{ow})^{0.77}$ [16], where f_{chp} and L_p are respectively the volumetric fractions of carbohydrate and lipid of the potato tissue and k_{chw} is the pesticide's carbohydrate-water partition coefficient [21]. As an approximation, we thus assume k_{chw} to be 0.1 for compounds with $\log k_{ow} < 0$; 0.2 for $0 \leq \log k_{ow} < 1.0$; 0.5 for $1.0 \leq \log k_{ow} < 2.0$; 1 for $2.0 \leq \log k_{ow} < 3.0$ for; 2 for $3.0 \leq \log k_{ow} < 4.0$ and 3 for $\log k_{ow} \geq 4.0$ [21]. The tortuosity factor is calculated using the method of Millington and Quirk, see [22,23], and is given by $\tau_w = (f_w)^{10/3} / (f_w + f_a)^2$. The pesticide diffusivity in soil solution, D_w $(\mathrm{m^2 day^{-1}})$, was estimated by $D_w = \dfrac{4.93\times 10^{-6} T_w \sqrt{\phi_w w_m}}{\xi_w (v_m)^{0.6}}$, where $(T_w = 298^{\circ}\mathrm{K})$ is the average soil temperature, $\phi_w = 2.6$ is an association term for the solvent (water), $w_m = 18\mathrm{g\ mol^{-1}}$ is the molar mass of water, $\xi_w = 8.9\times 10^{-1}\mathrm{cp}$ is the water viscosity and v_m $(\mathrm{cm^3\ mol^{-1}})$ is the molar volume of the pesticide, see [23].

Pesticide concentration in soil solution was described by a dispersion-advection equation (DAE) given by

$$D_e \frac{\partial^2 C_w}{\partial z^2} - v_w \frac{\partial C_w}{\partial z} - R_f \left(\frac{\partial C_w}{\partial t} + k_s C_w \right) = 0 \qquad (2)$$

where D_e ($\mathrm{m^2 day^{-1}}$) is the soil solution's coefficient of effective dispersion, $C_w = C_w(z,t)$ ($\mathrm{mg\ L^{-1}}$) is the pesticide concentration in soil solution, R_f is the retardation factor of pesticide in soil, v_w ($\mathrm{m\ day^{-1}}$), is the speed of water flow in soil pores, ρ_w ($\mathrm{kg\ L^{-1}}$) is the wet density of the soil and k_s ($\mathrm{day^{-1}}$) is the pesticide's degradation rate in soil, which in turn is estimated by $k_s = \ln(2)/t_{1/2}$, where $t_{1/2}$ (day) is the pesticide's half-life in the soil. The retardation factor was estimated by $R_f = 1 + \dfrac{\rho_s f_{oc} k_{oc} + f_a k_{aw}}{f_w}$.

According to Jury et al (1992), the coefficient of effective dispersion is the sum of the pesticide's molecular diffusion in soil solution plus the soil solution's hydrodynamic dispersion, estimated by $D_e = \tau_w D_w + \alpha_s v_w$, where f_w is the volumetric fraction of water in soil in the field capacity and α_s (m) is a factor expressing water dispersion in the soil. The term αv_w ($\mathrm{m^2 day^{-1}}$) is the coefficient of hydrodynamic dispersion and τ_w is a tortuosity coefficient, see [23,24].

The thin top layer of the soil that initially contains the pesticide is considered as part of the soil profile and its existence is incorporated to the initial conditions. The modelled soil profile has a form of $z = 0$ up to $z = \varepsilon$. The initial conditions are then given by

$$C_w(z,0) = \frac{10^{-4} \times ad}{\varepsilon(\rho_s k_{OC} f_{OC} + f_w)}, \quad 0 < z < \varepsilon \qquad (3)$$

and

$$C_w(z,0) = 0, \quad \varepsilon < z < +\infty \qquad (4)$$

where ad ($\mathrm{g\ ha^{-1}}$) is the pesticide application dose and ε (m) is the width of the top layer of soil surface that describes the initial area, where takes place the incorporation of pesticides applied to the soil. The model given by Equation 2 needs two boundary conditions; in the definition of the boundary condition, it is assumed that the water added on top of the soil is free from pesticides and that there is not a concentration gradient in the soil layer of infinite depth. Then, the boundary conditions for Equation 2 are given by

$$v_w C_w(0,t) - D_e \frac{\partial C_w(0,t)}{\partial z} = 0, \quad t \geq 0 \qquad (5)$$

and

$$\frac{\partial C_w(+\infty,t)}{\partial z} = 0, \quad t \geq 0 \qquad (6)$$

where all the terms have already been defined. Numerical solutions of the coupling between the pesticide concentration in potatoes, as given by the ODE defined by Equation 1, and the pesticide concentration in soil solution as given by the DAE, defined by Equations 2-6, were obtained by using a finite difference method similar to those used by Contreras and co-workers [25].

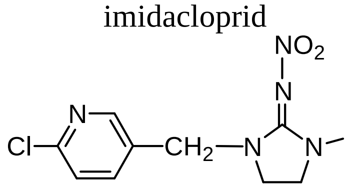
2.1.2 Input data

We have selected the imidacloprid insecticide to simulate the effects that pesticide leaching and degradation in the soil have upon pesticide accumulation in potatoes. Imidacloprid (1-[(6-chloro-3-pyridinyl)methyl]-N-nitro-2-imidazolidinimine) is a neonico-tinoid insecticide that acts biochemically as an antagonist by binding to postsynaptic nicotinic receptors in the central nervous system of insects. It is a systemic insecticide with translaminar activity and with contact and stomach action. Readily taken up by the plant, it is then distributed acropetally with good root-systemic action. Imidacloprid is one of the most widely used insecticides and it can be applied by soil injection, tree injection, application to the skin, broadcast foliar, ground application as granular or liquid formulation or as a pesticide-coated seed treatment. In potatoes, it is recommended for the control of aphids (*Myzus persicae*), thrips (*Thrips palmi*), beetles (*Diabrotica speciosa*) and other insects. It is also effective against insects that attack barley, beans, broccoli, cabbage, cauliflower, chicory, chrysanthemum, citrus, coffee, corn, cotton, cucumbers, eggplant, garlic, gerbera, grapes, kale, lettuce, melon, oats, onions, peanuts, peppers, pineapple, poinsettia, pumpkin, rice, sorghum, soybean, squash, sugar cane, sunflower, tobacco, tomatoes, watermelon and wheat. Doses used for foliar applications are between 25-100 g ha^{-1}, while for seed treatment the doses are 50-175 g/100 kg^{-1} for seeds in general, and 350-700 g/100 kg^{-1} for cotton seeds [26]. Metabolites of imidacloprid have a broad range of toxicities, with some of them showing stronger insecticidal activity than the parent compound and several of them demonstrating chronic toxicity to honeybees in dosing studies, see [27,28].

Imidacloprid has been reported to persist in different concentrations in stems and roots of plants, depending on the application method [29]. Thus, the pesticide can be an important hazard to the environment because it is categorized as moderately toxic and with a high potential to leach into groundwater [30,31]. Imidacloprid can persist for a period longer than 90 days under dry or cold conditions, and is moderately to highly mobile in soils with low clay or organic matter content. Because it does not adsorb strongly to soil particles and has a lengthy half-life of more than 90 days and moderate to high solubility in water (610 mg L^{-1}), it has a high potential for groundwater contamination [32-35]. Imidacloprid was found in fresh potatoes sold in farmers' markets in Alberta, Canada, at concentrations ranging from 15-31 $\mu g\ kg^{-1}$ [15].

Table 1 presents the physicochemical properties of imidacloprid necessary for the model given by Equations 1-6 to simulate both the uptake of insecticide imidacloprid by potatoes and the lixiviation in soil. Table 2 presents the values of potato and soil which were used in numerical simulation by Equations 1-6. In these simulations an implicit numerical scheme was used similar to the one used by Freijer and co-workers [24], with an integration time step of 5.0×10^{-3} days and an integration depth step of 1.0×10^{-2} meters. In the initial conditions given by Equations 3-4, the depth of the superficial soil layer was assumed to be $\varepsilon = 1.0\times10^{-2}$ meters, in a soil profile of 1.0 meter of depth ($0.01 \le z \le 1.0$). The total time adopted for the simulation was 120 days, which corresponds to the longest period until potato harvest, after pesticide is applied in the soil on day zero, and an initial imidacloprid concentration of 100g ha^{-1} (Equation 3) was assumed for the soil solution.

Table 1. Imidacloprid physicochemical characteristics.

Common name	imidacloprid
Molecular structure	
CAS RN	138261-41-3
Field use and class	Insecticide and neonicotinoid
Chemical Abstracts name	1-[(6-chloro-3-pyridinyl)methyl]-N-nitro-2-imidazolidinimine
IUPAC name	1-(6-chloro-3-pyridylmethyl)-N-nitroimidazolidin-2-ylideneamine
Molecular formula	$C_9H_{10}ClN_5O_2$
Half-life in the soil: $t_{1/2}$	120 days
Molar volume: v_m	160.1 $cm^3\ mol^{-1}$
Molecular weight: P_m	255.67 g mol^{-1}
Octanol-water partition coefficient: K_{ow}	3.71 ($\log K_{OW} = 0.57$)
Organic carbon partition coefficient: K_{oc}	$k_{OC} = 10^{(0.1+0.81\log K_{OW})}$ L kg^{-1}
Vapor pressure: P_v	4.0×10^{-10} Pa
Water solubility: S_w	610 g m^{-3}

Sources: Available at https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf; http://www.syrres.com/what-we-do/databaseforms.aspx?id=386 and [26].

Table 2. Physicochemical parameters for potato plants and soil applied to the ODE-DAE model to estimate concentrations of pesticides in potatoes.

Parameter	Symbol	Value	Unit
potato water volumetric content[a]	w_p	0.778	L L^{-1}
potato lipid volumetric content[a]	L_p	0.001	L L^{-1}
potato carbohydrate volumetric content[a]	f_{chp}	0.154	L L^{-1}
pesticide dissipation in potato[a]	k_p	0.142	day^{-1}
potato density[b]	ρ_p	1.4	kg L^{-1}
average potato sphere ray[a]	r_p	0.03	m
soil-organic carbon volumetric fraction[a]	f_{oc}	0.02	L L^{-1}
soil-water volumetric fraction[a]	f_w	0.25	L L^{-1}
soil-air volumetric fraction[a]	f_a	0.12	L L^{-1}
soil density on dry base[a]	ρ_s	1.1	kg L^{-1}
maximum depth of potato plants roots	δ_r	0.10	m
initial concentration of pesticide in soil solution	$C(0,0)$	1.0	mg L^{-1}
initial concentration of pesticide in potato	$C_p(0)$	0.0	mg kg^{-1}
water speed in soil pores	v_w	0.031	m day^{-1}
longitude of dispersion in the soil	α_s	0.005	m
soil porosity	σ_s	0.37	L L^{-1}
soil tortuosity factor	τ_w	0.183	-

[a]See [16]; [b]Available at http://www.starch.dk/isi/starch/tm5www-potato.asp

3. Numerical simulation, results and discussion

The value of octanol-water partition coefficient of 3.71 $(\log k_{ow} = 0.57)$ indicates that imidacloprid has a low lipid affinity. The value of organic carbon-water partition coefficient, 3.64 $L\,kg^{-1}$ (k_{OC}), indicates that imidacloprid has a low affinity with soil organic matter, which means that its translocation from soil solution to potato cannot be difficult. The value of 6.77×10^{-14} obtained for the air-water partition coefficient (k_{aw}) using data from Table 1, indicates that imidacloprid is not volatile at the temperature of 25°C [36]. The value of 2.60 for the pesticide uptake rate (k_u) indicates good imidacloprid mobility in the potato by diffusion [16]. The value of 0.81 for the potato to water partition coefficient (k_{pw}) indicates that imidacloprid has a moderate affinity with potato material, see [13,16].

The imidacloprid concentration in potatoes over time, as simulated by the ODE-ADE model, is illustrated in Figure 1. Initially, the compound concentration is null, then it increases continuously up to a maximum value, after which it decreases with time. This concentration pattern is due to the compartment system described by the ODE model and it was assumed for the pesticide in potato dissipation kinetic of first order, Equation 1. At the 6th day ($t_{\max} = 6.7$) after imidacloprid application at the first day ($t = 0$) to the soil, its concentration in potatoes reaches the simulated maximum value of $0.15\,\mathrm{mg\ kg^{-1}}$ ($C_p(t_{\max}) = 0.15\,\mathrm{mg\ kg^{-1}}$). In similar simulations with the azoxystrobin fungicide we found values for $t_{\max}$ and $C_p(t_{\max})$ of 43 days and $3.6\times10^{-3}\,\mathrm{mg\ kg^{-1}}$, respectively. Concentrations estimated by the ODE-ADE model are consistent with concentration values for imidacloprid and azoxystrobin that were observed experimentally in commercial potatoes in Alberta, Canada, by Thompson and co-workers [15].

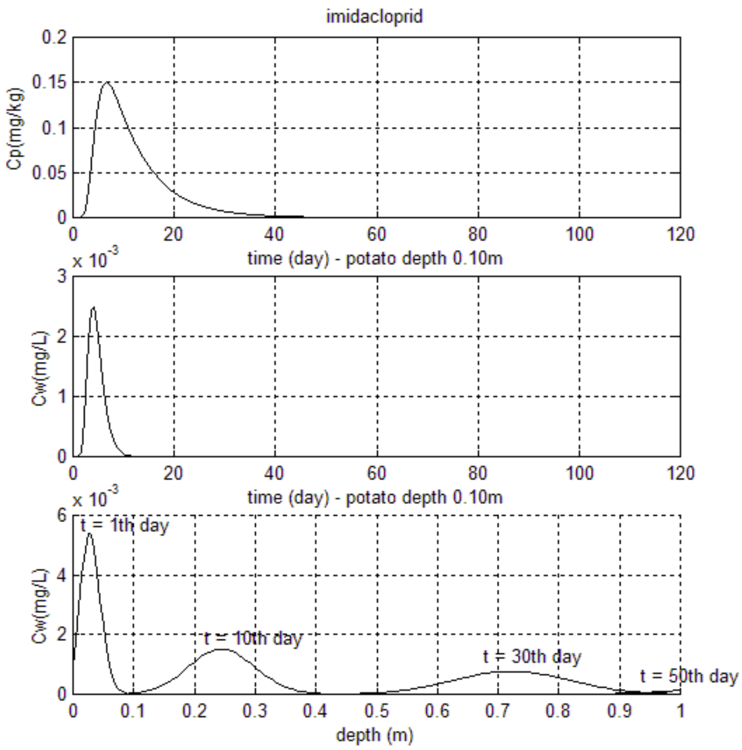


Figure 1. Concentrations along time of the imidacloprid insecticide in potato and soil, simulated by means of an ODE_ADE model.

Figure 1 presents imidacloprid concentrations resulting from simulations of the uptake by potatoes of imidacloprid in soil solution, $C_w(t)$, at the average depth of potatoes in the soil – 10cm $(\delta_r = 0.10\text{m})$. For depths between 0.0 and 1.0m and times $t=1$, $t=10$, $t=30$, $t=50$ days, Figure 1 presents concentrations of imidacloprid resulting from dispersion and advection of the solution along the soil profile. The overall pattern of imidacloprid concentrations along the soil profile indicates that potatoes located at depths of over 0.20m would be less exposed to absorbing imidacloprid from the soil solution. The concentration pattern along the soil profile will have an influence on imidacloprid uptake by potatoes.

3.1 ODE-ADE model sensitivity analysis

Data in Table 1 and Table 2, together with the numerical method programmed in Matlab®, were used to analyze the effect of the variation of a potato's average depth into the soil, δ_r (m), on the maximum concentration of imidacloprid in potatoes, $C_p(t_{\max})$, and on the time taken for the maximum concentration to occur in potatoes, $t_{\max}$. So, the model was executed for values of δ_r between 0.05m and 0.4m. Figure 2 presents values of $C_p(t_{\max})$ and $t_{\max}$ obtained by the ODE-ADE model for values of δ_r in $[0.05; 0.40]$. It can be observed in Figure 2 that values of $C_p(t_{\max})$ decline uniformly according to an apparent negative exponential pattern and that $t_{\max}$ grows linearly as the average depths of potatoes in soil, δ_r, increase, that is, potatoes that are deeper down in the soil have smaller values of maximum concentrations and these ones are reached at later times.

It is possible to carry out another sensitive analysis with the ODE-ADE model in Matlab® program to investigate the effect of the conjoint variations of the pesticide octanol-water partition coefficient and the pesticide half-life in soil, upon the maximum concentration of pesticide in potatoes and upon the maximum time concentration. For this, let potato and soil data be those of Table 1 and Table 2. The colour filled contour plots in Figure 3 and Figure 4 were obtained by conjoint varying of $\log k_{ow}$ in $[-1.0; 6.0]$ $(-1.0 \le \log k_{ow} \le 6.0)$ and half-life in $[1; 200]$ $(1 \le t_{1/2} \le 200$ days) and assuming $\delta_r = 0.12\text{m}$. It can be observed that the conjoint variation of the pesticide octanol-water partition coefficient and pesticide half-life in soil indicates that pesticides with $\log k_{ow} < 1.0$ and half-life longer than 20 days $(t_{1/2} > 20)$ present the highest maximum concentrations in potatoes (Figure 3). On the other hand, pesticides with $\log k_{ow} > 3.0$ and half-life longer than 20 days $(t_{1/2} > 20)$ reach maximum concentrations in potatoes at later times (Figure 4).

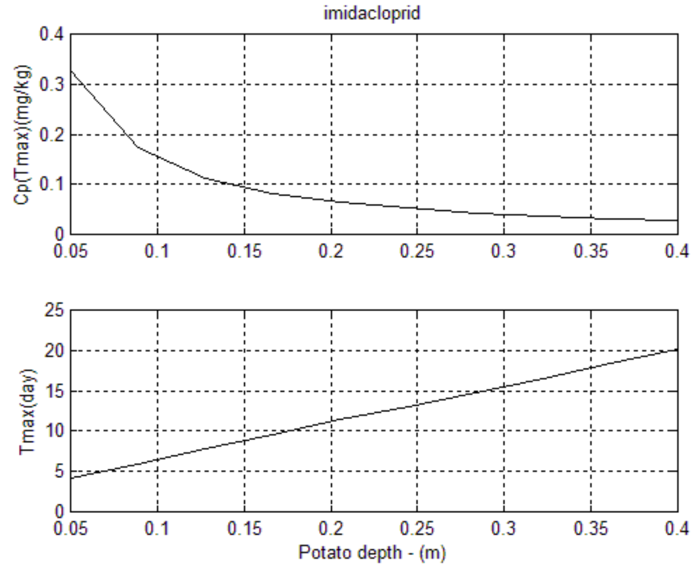


Figure 2. Sensitivity analysis of the maximum concentration $C_p(t_{\max})$ of the imidacloprid insecticide from soil solution in potato, and the time necessary to reach maximum pesticide concentration $t_{\max}$ in potato, simulated by means of an ODE_ADE model.

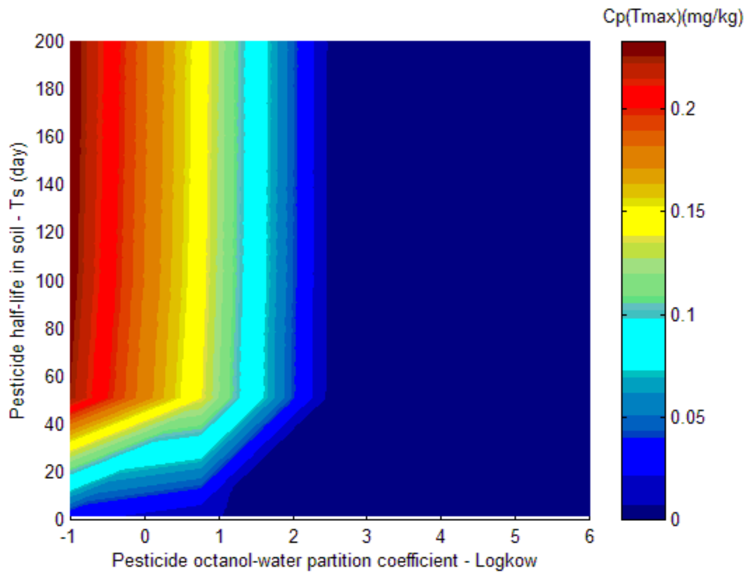


Figure 3. Color diagram representing the joint relation of pesticide octanol-water partition coefficient, $\log k_{ow}$, and pesticide half-life in soil, $t_{1/2}$, with the maximum pesticide concentration in potato, $C_p(t_{\max})$, simulated by means of an ODE-ADE model.

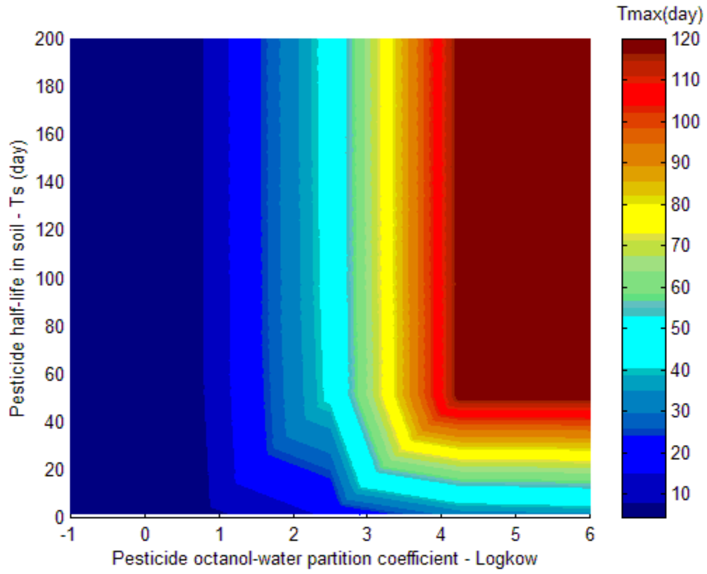


Figure 4. Color diagram representing the joint relation of pesticide octanol-water partition coefficient, $\log k_{ow}$, and pesticide half-life in soil, $t_{1/2}$, with the time necessary to reach maximum pesticide concentration in potato, $t_{\max}$, simulated by means of an ODE-ADE model.

4. Conclusions

The ODE-ADE model presented in this work allows estimation of pesticide concentrations in potato and in soil solution. Pesticides are unstable organic compounds that undergo degradation reactions in soils and can be taken up by potatoes from the soil solution through diffusion. The ODE-ADE model sensitivity analysis, regarding the pesticide octanol-water partition coefficient, the pesticide half-life in soil and the average depth of potatoes proved that soil depth affects the quantity of pesticide concentrations in potato and, consequently, affects the pesticide maximum concentration and the time it takes to reach maximum concentration. According to the model, potatoes in deeper layers may be more protected against contamination as much because they are exposed to lesser concentrations of pesticides that suffer dispersion when leached, as because such exposure occurs later on the crop cycle. Based on the model's results, was observed that values of the octanol-water partition coefficient and of the pesticide's half-life in soil have great influence upon the uptake of pesticides by potatoes. Specifically for imidacloprid, it reaches simulated maximum concentration of 0.15 *mg kg*$^{-1}$ ($C_p(t_{\max}) = 0.15$ mg kg^{-1}) in potatoes during 6th day ($t_{\max} = 6.7$) after application to the soil.

It is possible to develop agronomic strategies for both crop management and for use of pesticides in potatoes. It is even possible to define industrial goals, based on mathematical modelling, for the efficient formulation of pesticides that bring benefits to the soil environment and avoid pesticide uptake by potatoes. This modelling tool can be used as a computationally efficient aid to field study design, model calibration (changes in what input parameters have the greatest impact on model output), and to further our understanding of the physical mechanisms involved in pesticide uptake by potatoes and pesticide transport in soil.

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