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Numerical Simulation of Pesticide Propagation in Soil: Advection and Diffusion Modeling

Daniela Buske[1] Régis S. de Quadros[2]
Postgraduate Program in Mathematical Modeling, UFPel, Pelotas, RS
João G. P. Bandeira[3]
Control and Automation Engineering, UFPel, Pelotas, RS

Abstract. Pesticides play a crucial role in modern agriculture, enhancing crop yields and quality. However, their widespread use raises concerns about environmental pollution and human health risks. This study addresses these concerns by presenting a simulation model to predict the fate of pesticides in soil, considering various factors such as soil composition, water flow velocity, diffusion coefficients, and degradation rates. Through numerical simulation, the model demonstrates its capability to predict pesticide propagation over time and space, as well as illustrating the impact of different parameters, highlighting the importance of sustainable pesticide use practices. Overall, this study contributes to efforts aimed at developing effective pesticide management strategies and protecting the environment.

Keywords. Pesticides, Sustainable agriculture, Computational analysis, Numerical simulation, Advection-diffusion equation

1 Introduction

Pesticides, a category of substances that includes insecticides, fungicides, herbicides, rodenticides, molluscicides, and nematicides [12], are acknowledged for their substantial role in agricultural development, particularly highlighting the top three, which stand out as the most widely sold worldwide [7]. They are widely acknowledged for their ability to reduce agricultural product losses, thereby improving the yield and quality of food within the same cultivated surface areas in an economically viable manner [2, 3, 7, 12].

In Brazil, the increase in pesticide consumption is directly related to the historically conducted policies promoting commodity production by the Brazilian government. In 1991, the country used seven times fewer pesticides than the United States; however, by 2015, both countries consumed about 400.000 tons per year [4]. Nowadays, along with other countries like the USA and China, Brazil is one of the countries that consumes the most pesticides in the world [4–6, 8, 9].

Every year, three billion kilograms of pesticides are utilized globally, with only 1% effectively targeting insect pests on intended plants [12]. The substantial quantity of unused pesticides infiltrates non-target plants and environmental media, resulting in environmental pollution and adverse effects on human health [2–4, 7, 11, 12].

Predicting the fate of pesticides in the environment is essential to minimize adverse impacts beyond their application sites. Understanding chemical dynamics and pesticide residues present in plants and soil is essential to ensure food safety and protect the environment [1, 13]. Additionally,

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[1] danielabuske@gmail.com
[2] quadros99@gmail.com
[3] joaogabrielpbandeira@gmail.com

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information about the fate of pesticides in agriculture can inform governmental decisions, such as defining appropriate pre-harvest intervals to keep pesticide concentrations below the maximum residue limit over time [1].

Several simulation models have already been developed to provide a deeper understanding of plant-environment system characteristics and represent an effective approach to assess agricultural and environmental challenges related to pesticide use [1, 13]. These models assist in selecting suitable pesticides for specific soil, crop, and weather conditions, optimizing application rates and timing to protect crops, and identifying pesticides with high contamination potential for specific environmental compartments [13].

Choosing the most appropriate model hinges on several factors: the intended purpose of the study, the accessibility of input data, and the model's capacity to accurately represent physical and chemical processes through parametrization. These considerations collectively guide the decision-making process, ensuring that the selected model is well-aligned with the specific objectives and limitations of the study [2].

The objective of this work is to present a simulation model to predict the fate of pesticides in the environment, considering factors such as soil composition, water flow velocity, diffusion coefficients, and degradation rates.

2 Methodology

The model corresponds to an experiment where a soil-pesticide mixture is prepared with a known pesticide concentration. A layer of this mixture is positioned on top of a soil column that is already saturated with water. Subsequently, water is introduced at a constant rate to the top of the soil column, thereby prompting the transport of the pesticide from the upper layer. An investigation will be conducted on an advection-diffusion model with degradation evolution, based on [10], described as

$$R_f \frac{\partial C(x,t)}{\partial t} - D\frac{\partial^2 C(x,t)}{\partial x^2} + V\frac{\partial C(x,t)}{\partial x} + R_f k C(x,t) = 0\,, \tag{1}$$

where C is the solute concentration in $kg\,m^{-3}$, t is time in days (d), x is the spatial coordinate in meters (m), positive in the direction of soil depth, R_f is the retardation factor (dimensionless), D is the diffusion coefficient in $m^2\,d^{-1}$, V is the water flow velocity in $m\,d^{-1}$ and k is the degradation factor in d^{-1}.

The retardation factor is

$$R_f = 1 + \frac{\rho K_D}{\theta}\,, \tag{2}$$

where ρ is the density of dry soil in $kg\,m^{-3}$, $K_D = f_{oc}K_{oc}$ is the pesticide sorption coefficient in the soil in $m^3\,kg^{-1}$, f_{oc} is the organic carbon content in the soil, K_{oc} is the sorption coefficient of the pesticide to the organic carbon in the soil in $m^3\,kg^{-1}$ and θ is the volumetric water content in the soil. The diffusion coefficient is given by

$$D = \kappa D_0 + \alpha V \tag{3}$$

where D_0 is the diffusion coefficient in water in $m^2\,d^{-1}$, κ is the soil factor and α is the dispersal length in (m).

2.1 Initial and boundary conditions

For the boundary condition at $x = 0$, it is assumed that the water added at the top of the column is free of pesticides. Thus, it follows that

$$V\,C(0,t) - D\frac{\partial C(0,t)}{\partial x} = 0 \qquad , \qquad t > 0\,. \tag{4}$$

The layer at the top of the soil column, which initially contains the pesticide, is considered as part of the soil profile, and its presence is incorporated into the domain through the initial condition

$$C(x,0) = \begin{cases} C_0 & , \quad 0 < x \leq \varepsilon \\ 0 & , \quad \varepsilon < x < L \end{cases} \qquad , \tag{5}$$

where C_0 is the initial concentration, ε is the thickness of the layer that initially contains the pesticide in m and L is the length of the soil column in m.

The boundary condition at $x = L$, in order to indicate that there is no concentration gradient at the bottom of the soil column, can be given by

$$\frac{\partial C(L,t)}{\partial x} = 0 \qquad , \qquad t > 0\,. \tag{6}$$

2.2 Numerical Simulation

The model will be discretized using the Crank-Nicolson scheme, defining C_i^j as the approximation of $C(x,t)$ at x_i, t_j. Thus, the equation (1) is discretized as follows:

$$R_f\frac{C_i^{j+1} - C_i^j}{\Delta t} - \frac{D}{2}\left(\frac{C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}}{h^2} + \frac{C_{i+1}^{j} - 2C_i^{j} + C_{i-1}^{j}}{h^2}\right)$$
$$+ \frac{V}{2}\left(\frac{C_{i+1}^{j+1} - C_{i-1}^{j+1}}{2h} + \frac{C_{i+1}^{j} - C_{i-1}^{j}}{2h}\right) + \frac{R_f k}{2}(C_i^{j+1} + C_i^j) = 0. \tag{7}$$

Then, by defining the coefficients as

$$\alpha = -D - \frac{Vh}{2}, \tag{8}$$

$$\lambda = \frac{2R_f h^2}{\Delta t} + 2D + R_f k h^2, \tag{9}$$

$$\beta = -D + \frac{Vh}{2}, \tag{10}$$

$$\mu = -\frac{2R_f h^2}{\Delta t} + 2D + R_f k h^2, \tag{11}$$

the expression, for $i = 1, 2, 3 \ldots, n$ and $j = 0, 1, 2 \ldots$, becomes

$$\alpha C_{i-1}^{j+1} + \lambda C_i^{j+1} + \beta C_{i+1}^{j+1} = -\alpha C_{i-1}^j - \mu C_i^j - \beta C_{i+1}^j. \tag{12}$$

By discretizing the boundary conditions using the following one-sided forward finite difference formula

$$f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h}, \tag{13}$$

the equation (12), for $i = 1$, turns into

$$\left(\lambda + \frac{4D\alpha}{2Vh + 3D}\right) C_1^{j+1} + \left(\beta - \frac{D\alpha}{2Vh + 3D}\right) C_2^{j+1} = -\alpha C_0^j - \mu C_1^j - \beta C_2^j. \tag{14}$$

Furthermore, using the one-sided backward finite difference formula

$$f'(x) = \frac{f(x-2h) - 4f(x-h) + 3f(x)}{2h}, \tag{15}$$

the equation (12), for $i = n$, becomes

$$\left(\alpha - \frac{\beta}{3}\right) C_{n-1}^{j+1} + \left(\lambda + \frac{4\beta}{3}\right) C_n^{j+1} = -\alpha C_{n-1}^j - \mu C_n^j - \beta C_{n+1}^j. \tag{16}$$

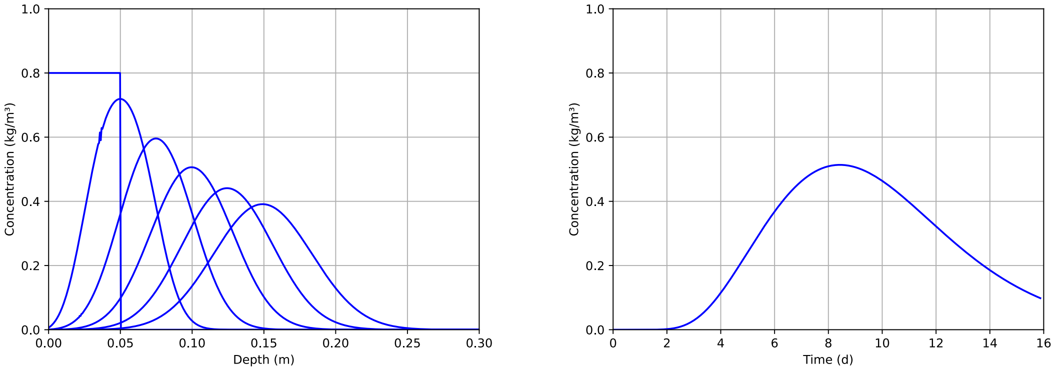
Numerical solutions are obtained by solving the system of equations (12), (14) and (16). A script was made in Python language for the simulation. The parameters used in the simulation are shown in Table 1, and are based on [10].

Table 1: Simulation parameters.

$L\ (m)$	$T_f\ (d)$	$C_0\ (kg\,m^{-3})$	f_{oc}	θ	R_f	h
0.3	16	0.8	0.01	0.4	3.1	0.3/512
$D\ (m^2\,d^{-1})$	$V\ (m\,d^{-1})$	$k\ (d^{-1})$	$K_{oc}\ (m^3\,kg^{-1})$	$\rho\ (kg\,m^{-3})$	$\varepsilon\ (m)$	Δt
1×10^{-4}	0.04	0.01	0.06	1400	0.05	16/128

3 Results and Discussion

In Figure 1a, the plot of $C(x,t)$ is presented for a temporal variation using $t = 0, 3, 6, 9, 12,$ and 15 days. Additionally, Figure 1b depicts the plot of $C(x,t)$ for $x = 0.1\,m$. It's evident that over time, the concentration diminishes due to factors such as degradation, and the shape of the curve broadens, primarily due to diffusion, among other contributing factors.

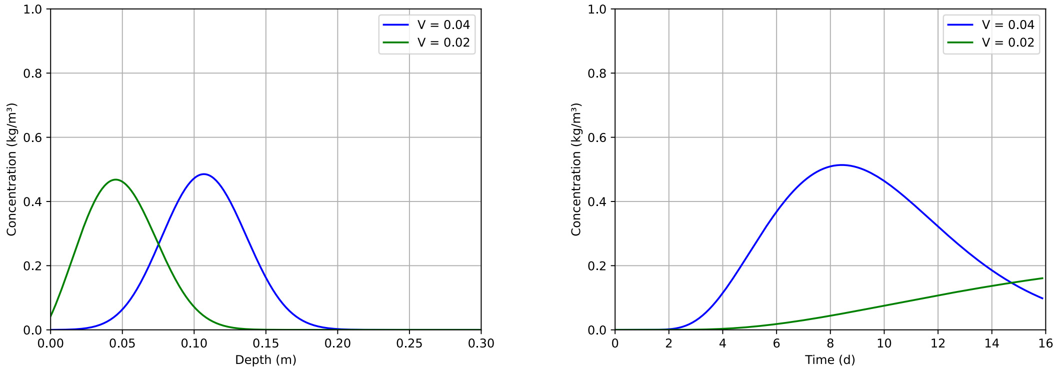


(a) (b)

Figure 1: Numerical solution of $C(x,t)$ for (a) $t = 0, 3, 6, 9, 12, 15$ days and for (b) $x = 0.1$ m using the parameters from Table 1. Source: authors.

It's possible to explore the influence of parameters in the simulation. For instance, Figure 2 demonstrates the effect of the water flow velocity V. It can be inferred that a higher velocity propagates the pesticide faster and deeper through the soil.

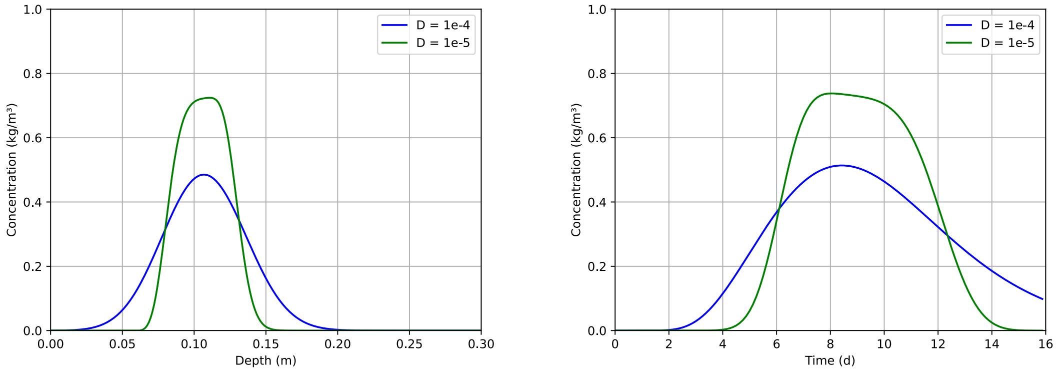
Similarly, Figures 3 and 4 illustrate the impact of the diffusion coefficient D and the degradation factor k. A higher diffusion coefficient results in the pesticide being more dispersed, leading to a lower maximum concentration at each depth. This effect contrasts with changes in velocity alone, where such reduction in maximum concentration doesn't occur. Also, it is reasonable to assume that a higher degradation factor accelerates the decrease in pesticide concentration, preventing it from reaching higher levels.



(a)

(b)

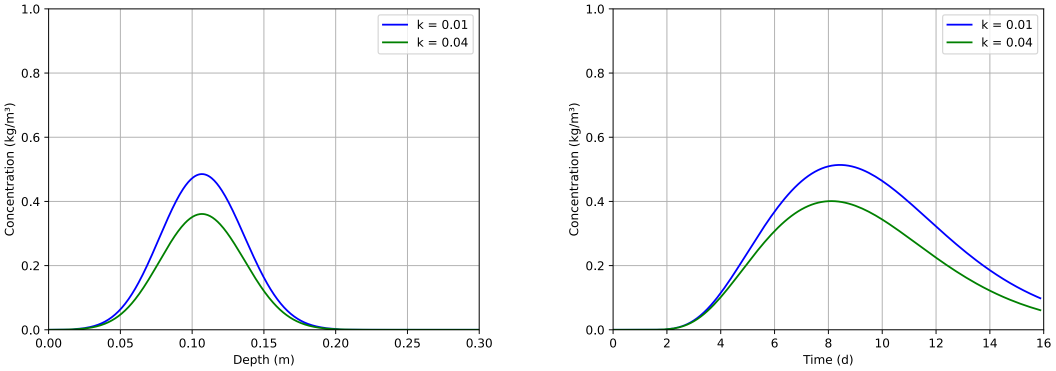
Figure 2: Impact of water flow velocity V for (a) $t = 10$ days and for (b) $x = 0.1$ m. Source: authors.



(a)

(b)

Figure 3: Impact of diffusion coefficient D for (a) $t = 10$ days and for (b) $x = 0.1$ m. Source: authors.



(a) (b)

Figure 4: Impact of degradation factor k for (a) $t = 10$ days and for (b) $x = 0.1$ m. Source: authors.

4 Conclusion

The simulation model presented in this study offers a valuable tool for understanding the dynamics of pesticide movement in soil and its potential impact on the environment. By considering various parameters such as soil composition, water flow velocity, diffusion coefficients, and degradation rates, the model is able to predict pesticide propagation over time and space, offering valuable information for decision-making in agriculture and environmental management.

By optimizing application rates, timing, and selection of pesticides based on soil and weather conditions, it is possible to mitigate environmental pollution and ensure food safety. Future research could focus on refining the model's parameters and validation against experimental data to enhance its predictive accuracy and applicability in real-world scenarios. Overall, this study contributes to the ongoing efforts to develop effective strategies for pesticide management and environmental protection.

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References

[1] Q. An, Y. Wu, D. Li, X. Hao, C. Pan, and A. Rein. "Development and application of a numerical dynamic model for pesticide residues in apple orchards". In: **Pest Management Science** 78.6 (2022), pp. 2679–2692. DOI: `10.1002/ps.6897`.

[2] M. Centanni, G. F. Ricci, A. M. De Girolamo, G. Romano, and F. Gentile. "A review of modeling pesticides in freshwaters: Current status, progress achieved and desirable improvements." In: **Environmental Pollution** 316 (2023), p. 120553. ISSN: 0269-7491. DOI: `10.1016/j.envpol.2022.120553`.

[3] J. P. Cunha. “Simulação da deriva de agrotóxicos em diferentes condições de pulverização”. In: **Ciencia E Agrotecnologia - CIENC AGROTEC** 32 (Oct. 2008). DOI: `10.1590/S1413-70542008000500039`.

[4] V. Daufenback, A. Adell, M. Mussoi, A. Furtado, S. Santos, and D. Veiga. “Agrotóxicos, desfechos em saúde e agroecologia no Brasil: uma revisão de escopo”. In: **Saúde em Debate** 46 (July 2022), pp. 482–500. DOI: `10.1590/0103-11042022e232`.

[5] M. T. Frota and C. E. Siqueira. “Agrotóxicos: Os Venenos Ocultos na Nossa Mesa”. In: **Cadernos de Saúde Pública** 37.2 (2021). DOI: `10.1590/0102-311x00004321`.

[6] S. Garcia and T. Lara. “O impacto do uso dos agrotóxicos na saúde pública: revisão de literatura”. In: **Saúde e Desenvolvimento Humano** 8 (Mar. 2020), p. 85. DOI: `10.18316/sdh.v8i1.6087`.

[7] F. Jacquet, M. Jeuffroy, J. Jouan, E. Le Cadre, I. Litrico, T. Malausa, X. Reboud, and C. Huyghe. “Pesticide-free agriculture as a new paradigm for research”. In: **Agronomy for Sustainable Development** 42.1 (Jan. 2022), p. 8. DOI: `10.1007/s13593-021-00742-8`.

[8] C. V. Lopes and G. S. Albuquerque. “Agrotóxicos e Seus Impactos na saúde humana e ambiental: Uma revisão sistemática”. In: **Saúde em Debate** 42.117 (June 2018), pp. 518–534. DOI: `10.1590/0103-1104201811714`.

[9] J. Medeiros, R. Acayaba, and C. Montagner. “A química na avaliação do impacto à saúde humana diante da exposição aos pesticidas”. In: **Química Nova** 44 (Jan. 2021). DOI: `10.21577/0100-4042.20170699`.

[10] P. Pulino. **Métodos de Diferenças Finitas: Aspectos Teóricos, Computacionais e Aplicações**. July 2008.

[11] F. H. M. Tang, M. Lenzen, A. McBratney, and F. Maggi. “Risk of pesticide pollution at the global scale”. In: **Nature Geoscience** 14.4 (Apr. 2021), pp. 206–210. ISSN: 1752-0908. DOI: `10.1038/s41561-021-00712-5`.

[12] M. Tudi, H. D. Ruan, L. Wang, J. Lyu, R. Sadler, D. Connell, C. Chu, and D. T. Phung. “Agriculture Development, Pesticide Application and Its Impact on the Environment”. In: **International Journal of Environmental Research and Public Health** 18.3 (2021). ISSN: 1660-4601. DOI: `10.3390/ijerph18031112`.

[13] R. J. Wagenet and P. S. C. Rao. “Modeling Pesticide Fate in Soils”. In: **Pesticides in the Soil Environment: Processes, Impacts and Modeling**. John Wiley Sons, Ltd, 1990. Chap. 10, pp. 351–399. ISBN: 9780891188612. DOI: `10.2136/sssabookser2.c10`.