BALANCING HEALTH AND SUSTAINABILITY: OPTIMIZING INVESTMENTS IN ORGANIC VS. CONVENTIONAL AGRICULTURE THROUGH PESTICIDE REDUCTION

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Balancing Health and Sustainability: Optimizing Investments in Organic vs. Conventional Agriculture Through Pesticide Reduction

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Abstract

This paper investigates the trade-offs between organic and conventional farming methods, focusing on their respective impacts on health, environmental sustainability, and economic outcomes. Our contributions are twofold. First, we develop a theoretical model based on an optimal control problem to examine the dynamic allocation of investments in organic versus conventional agriculture. This model incorporates critical social factors such as the environmental and health costs associated with the use of pesticides in conventional farming and the long-term social benefits of organic practices. Second, we estimate the key parameters of the model using French data on pesticide levels in groundwater and the costs of the treatments required to ensure safe and potable water for the population. The empirical results provide insights into the economic and environmental implications of shifting investments towards organic farming. By comparing theoretical and empirical results, key insights have been identified, regarding the interplay between the social costs of pesticide exposure, its spatial distribution, and the design of mitigation efforts. The optimal policy suggested, underscores the necessity of targeting localized areas of high pesticide concentration with intensified effort to minimize adverse health and environmental impacts. Furthermore, our model advocates for a balanced distribution of effort and emphasizes the efficacy of early intervention strategies. Failure to adhere to optimal effort levels could significantly increase future effort, and so the costs, required to achieve policymaker targets.

JEL Classification: C60, Q50, Q10

Keywords: Organic agriculture, Pesticide, Pollution, Optimal control, Parameter estimation

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1 Introduction

The intersection of health, sustainability, and agriculture has become a focal point of global discourse as nations grapple with the dual challenges of feeding growing populations and addressing environmental degradation. Agriculture is not only central to food security but also a major determinant of public health outcomes and environmental sustainability. As such, the choice between organic and conventional farming systems has far-reaching implications for global food systems, human well-being, and ecological resilience.

Organic agriculture is often celebrated for its environmentally friendly practices, such as reducing chemical pollution, preserving soil health, and enhancing biodiversity. It is also associated with producing food that is perceived to be safer and healthier due to the absence of synthetic pesticides and fertilizers. However, these benefits often come at the cost of lower yields and higher production expenses, raising questions about its scalability, affordability, and accessibility—particularly in regions where food insecurity remains a pressing issue. In contrast, conventional farming, characterized by its reliance on synthetic inputs and advanced technologies, offers higher productivity and cost efficiency but poses significant risks, including pesticide-related health issues, soil degradation, water contamination, and greenhouse gas emissions.

This paper analyzes the complex trade-offs between organic and conventional farming methods, focusing on their respective impacts on health, environmental sustainability, and economic outcomes. These trade-offs are not merely theoretical but deeply practical, influencing decisions regarding investment, policy design, and consumer behavior. Policymakers have been aware of potential side-effects of chemicals used in conventional practices; however, the literature suggests that their effects are still debated and unknown, especially when the long-term ones are considered. This is the case of atrazine, one of the most used herbicides in conventional production, which is still highly present in the European groundwater even if it was banned in 2004 due to its persistence and slow degradation. Exposure to atrazine through water and food consumption cause harmful health effects, primarily endocrine disruption and reproductive development issues with long-term societal implications. Since the 1970s, infertility rates have risen significantly and nowadays one in six individuals worldwide is concerned, according to the WHO [2023]. Obviously, chemical environmental exposures such as atrazine, along with lifestyle and social factors, are at the heart of this major public health issue. The negative effects of atrazine on fertility threaten economic growth, health systems, and pension sustainability, particularly in developed nations with aging populations. Crafting agricultural policies that balance competing priorities while advancing sustainability is a critical element.

Our contributions are twofold. First, we develop a theoretical framework grounded in an *optimal control model* to examine the dynamic allocation of investments between organic and conventional agriculture. This model incorporates critical factors such as including the costs of transitioning from conventional to organic agriculture, the social benefits of this shift, and the long-term consequences of residual pollution from conventional farming for future generations. By formalizing these relationships, the model provides a structured approach to understanding the interplay between short-term economic efficiency and long-term sustainability outcomes. Second, we estimate the key parameters of our theoretical model using French data on atrazine levels in groundwater and the costs of the treatments required to ensure safe and potable water for the population. France, as a leading agricultural producer in Europe, provides a compelling case study for examining these dynamics due to its diverse farming practices, strong policy focus on sustainability, and growing consumer demand for organic products.

Our model aims at minimizing pesticide-related social costs, such as water treatment and health, by reallocating investments to organic agriculture and reducing pesticide levels. Empirical evidence highlights a clear relationship between the social costs of pesticide exposure and its spatial concentration. Higher social costs tend to motivate greater efforts to reduce pesticide levels. Optimally allocating these efforts helps mitigate localized contamination hotspots, promoting a more uniform distribution of pesticide concentrations and delivering significant environmental benefits. The model also reveals diminishing returns, indicating that a balanced spatial allocation of effort maximizes overall effectiveness. Finally, early intervention of policymaker results in greater overall reductions of the diffusion of pesticides. Together, these actions contribute to offer an actionable framework for optimized agricultural policies to balance health, environmental, and economic goals.

Our findings underscore the importance of designing policies that account for both the immediate and long-term impacts of agricultural investments. By aligning public and private resources with health and sustainability goals, it is possible to create a more resilient and equitable global food system-one that meets the needs of the present without compromising the ability of future generations to thrive.

The remainder of the paper is organized as follows. Section 2 provides an overview of the existing literature, summarizing pivotal studies and pointing out the gaps this work aims to fill. Section 3 introduces the diffusion model, which explains how pesticides spread over time and space in interconnected groundwater systems. Section 4 lays out the optimal control problem. Section 5 describes the dataset we use, based on French atrazine pesticide data from 2016 to 2023. Section 6 presents the econometric methods used to estimate the parameters of the diffusion model. Finally, Section 7 discusses the implications of our findings for policies that promote sustainable farming and environmental conservation, bringing the paper to a close.

2 Literature Review

2.1 Organic vs. conventional agriculture

Organic agriculture is a farm management and food production system that enhances and preserves environmental resources and uses natural substances and processes [EU, 2018]. It is generally antithetical to conventional agriculture which, in this context, is used as a conterpoise: it represents farming and food production practices that, contrary to the organic one, are based on the use of synthetic fertilizers and pesticides to maximize crop yields [de Ponti et al., 2012, Sumberg and Giller, 2022].
Conventional modern agriculture, with its reliance on chemical inputs like fertilizers and pesticides, has significantly boosted global food production. However, the industrial approach towards agriculture and the use of agrochemicals pose serious environmental and human health risks [Hedlund et al., 2020]. The concept of an alternative, more bio-oriented approach to agriculture emerged in Germany in the late 1920s. Inspired by Rudolf Steiner's lectures on biodynamic products, farmers established Demeter, an association focused on marketing products obtained using soil manuring and astrological scheduling. In the same period of time, in India, Sir Albert Howard developed a composting system for soil and crop health based on the so-called "Law of Return", which emphasizes recycling organic waste to maintain soil fertility [Conford, 2002, Gomiero et al., 2011]. The term "organic farming" was only introduced in 1940 in Walter Northbourne's book "Look to the land", which described farming as a holistic, biologically complete process emphasizing nutrient recycling and continuous biological interactions. Since the 1990s, the organic farming movement has gained significant attention. Internationally, organic farming is officially recognized by the Codex Alimentarius Commission (CAC), FAO and WHO, which provides guidelines for organic food, from production to marketization. The first EU regulation on organic farming dates back to 1991 with the EEC [1991], introducing regulations and standards for organic products in terms of use of pesticides, artificial fertilizers in crops, as well as hormones and antibiotics in livestock [Gomiero et al., 2011].
Today, organic farming is a fast-growing, well-recognized system, appreciated for its multiple benefits that it guarantees over conventional farming. It is known that the intensive application of chemicals used in conventional farming settings has contributed to increased food production in smaller areas and helped address global food demand, helping farmers economically by lowering the total farm production cost. Nevertheless, it caused a loss of organic carbon in soil, environmental pollution, loss of biodiversity, and adverse climate change due to the intensive use of land and the substances on which it relies. Instead, organic farming addresses these issues by producing similar to higher quality food while protecting the environment. In fact, in terms of nutritional composition, products of organic farming present slightly better composition, with more antioxidants, omega-3 fatty acids, vitamin C and lower cadmium levels, saturated fatty acids Huber et al. [2011], Barański et al. [2014], Średnicka Tober et al. [2016], Reganold and Wachter [2016]. However, Smith-Spangler et al. [2012] found no macronutrient differences between organic and conventional foods, except for higher phosphorus and the aforementioned micronutrients in organic products, conferring a marginal nutritional advantage.
Evidence linking organic food consumption to direct health outcomes is limited but growing. A systematic review by Vigar et al. [2020] managed to identify a link between organic food intake and reduced risk of obesity, infertility and allergic sensitization, pre-eclampsia, and non-Hodgkin lymphoma with the first three being linked to higher pesticides intake from conventional agriculture products. However, both Vigar et al. [2020] and Brantsæter et al. [2017] did not find studies demonstrating strong, direct health benefit from organic diets and no significant differences in clinical outcomes, like allergies or infections, but they as well recognized the benefit coming from a lower exposition to pesticides.

By substantially reducing agrochemical use, organic farming mitigates the adverse health effects and environmental impacts of pesticide exposure, thereby decreasing associated societal costs and supporting biodiversity conservation [Shennan et al., 2017, de la Cruz et al., 2023, Popp et al., 2013]. For example, a study of preschool children found that those consuming organic diets had significantly lower concentrations of organophosphorus pesticide metabolites in their urine compared to children on conventional diets [Curl et al., 2003]. However, organic farms still apply pesticides, primarily using biopesticides with minimal human and environmental risks. In Europe, 55% of conventional pesticides contain health or environmental hazard statements, compared to only 3% of organic pesticides [Benbrook et al., 2021, Burtscher-Schaden et al., 2022].

While beneficial, organic agriculture has limitations. A meta-analysis conducted by Seufert et al. [2012] of 66 studies revealed that organic yields are, on average, 25% lower than conventional yields, with significant variation between crop types (e.g., cereals show larger gaps than legumes). Conversely, Ponisio et al. [2015] suggest that the yield gap narrows to 9–20% when organic systems are optimized with best practices, such as crop rotation and cover cropping. The literature indicates that conventional agriculture generally outperforms organic agriculture in crop yield. Consequently, the lower yields of organic agriculture require increased land use, potentially contributing to habitat loss. Although organic systems reduce chemical runoff and environmental impacts while fostering biodiversity and improving soil organic matter, land efficiency remains a critical trade-off in their environmental footprint [Tuck et al., 2014, Gattinger et al., 2012, Meier et al., 2015].

Furthermore, its higher production costs can make food less affordable. A meta-analysis of 40 studies by Crowder and Reganold [2015] found that organic foods are 20–40% more expensive than conventional, with premiums highest for fruits and vegetables (30–50%) and lower for dairy and grains (15–25%). The socio-economical implications of such drawback are not negligible as for consumers, premium prices restrict access, particularly for low-income households, reinforcing food inequality. The market growth of organic products could lead to higher economies of scale, and therefore a possible reduction of existing price gaps. Researchers such as Meemken and Qaim [2018] suggest that a balanced combination of best practices from both systems could lead to a more sustainable and cost-effective approach to agriculture. Tuomisto et al. [2012] echoes him suggesting further research efforts and policies to foster synergies between organic and conventional farming systems to minimize their combined environmental impact.

2.2 Impact of Pesticides on Health

The relationship between pesticide exposure and human health has been a subject of extensive research and growing concern due to its profound implications. Pesticides, including insecticides, herbicides, and fungicides, are widely used in agriculture to control pests and increase crop productivity. However, their chemical nature often poses significant risks to human health, particularly when exposure occurs through contaminated food, water, air, or occupational settings [Ali et al., 2021, Poudel et al., 2020, Zhou et al., 2024]. Numerous studies indicate that chronic exposure to pesticides can lead to a range of adverse health effects, including neurological disorders, respiratory issues, reproductive harm, and even cancer. For instance, organophosphates, a common class of pesticides, have been associated with neurodevelopmental delays and cognitive impairments in children, as evidenced by a longitudinal study conducted in California [Eskenazi et al., 2007], which highlighted that prenatal exposure to these chemicals resulted in lower IQs and attention deficits.

Similarly, glyphosate, a widely used herbicide, has been classified as probably carcinogenic by the International Agency for Research on Cancer (IARC) in 2015, following evidence of its association with non-Hodgkin lymphoma in agricultural workers [Portier et al., 2016].

Legal cases, such as rulings where individuals have been awarded significant damages after developing health issues linked to pesticide exposure, highlight the serious legal and health-related implications associated with these chemicals. Additionally, pesticide residues in food and water have raised concerns about endocrine disruption, as studies have shown that certain pesticides mimic or block hormones, causing developmental and reproductive disorders. Recent studies also revealed that exposure to chlorpyrifos, even at low levels, could disrupt the endocrine system and impair fetal growth [Ubaid ur Rahman et al., 2021].

The health risks are exacerbated in developing countries, where regulations are often lax, and farmers lack access to protective equipment, leading to acute poisoning incidents. According to the World Health Organization (WHO), pesticide poisoning accounts for nearly 200,000 deaths annually, primarily in low- and middle-income countries [Boedeker et al., 2020]. These elements highlight the significant health risks related to pesticide exposure.

2.3 Diffusion models with reaction-diffusion equations

Since the use of pesticides is the key factor distinguishing the two different farming methods, we will concentrate on how these chemicals disperse and impact the environment, detailing their diffusion processes.

Diffusion models and differential equations are essential in studying the spread of pollutants in environmental systems. Understanding pollution diffusion is critical for analyzing how contaminants move through geographical areas, influenced by factors such as wind patterns, water currents, and human activities [Boucekkine et al., 2019, 2022, 2023].

Rather than accumulating in one location, pollutants disperse spatially, a phenomenon particularly significant for persistent contaminants such as radiation and chemicals, which remain active over long periods. This calls for spatial models that integrate both spatial and temporal dimensions to assess their long-term impacts on ecosystems and human health [Augeraud-Véron et al., 2019].

When considering continuous space and time dimensions, these equations take the form of reaction-diffusion models. Reaction-diffusion equations are a class of partial differential equations (PDEs) that describe the combined effects of diffusion and reaction processes [Xepapadeas, 2010, Aniţa et al., 2015, Camacho and Cornet, 2020, La Torre et al., 2021, De Frutos et al., 2021, La Torre et al., 2022]. These equations are widely used to model the spread of pollutants in natural and engineered environments, such as rivers, air, and soil. The general form of a reaction-diffusion equation is:

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = D\nabla^2 u(\mathbf{x},t) + R(u(\mathbf{x},t),\mathbf{x},t), \tag{1}$$

where: $u(\mathbf{x},t)$ is the pollutant concentration as a function of position $\mathbf{x}$ and time t, D is the diffusion coefficient, representing the rate of spreading, $\nabla^2 u(\mathbf{x},t)$ is the Laplacian operator (spatial diffusion), $R(u(\mathbf{x},t),\mathbf{x},t)$ is the reaction term, which accounts for processes like chemical reactions, degradation, or external sources. Here we list some applications of reaction-diffusion models.

- *Pollutant Spread in Rivers.* In a one-dimensional river system, the pollutant is transported longitudinally (x-direction). The reaction-diffusion equation becomes:

  $$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} - ku(x,t) + S(x,t), \tag{2}$$

  where: D is the diffusion coefficient in the river, k is the decay constant representing pollutant degradation, $S(x,t)$ is the source term describing pollutant input [Xing et al., 2024, Zhou and Huang, 2022, Deng and Huang, 2024].

- *Air Pollution Dispersion.* For air pollution, the spread is often modeled in three spatial dimensions, with advection (transport due to wind) and diffusion. The equation is:

  $$\frac{\partial u(\mathbf{x},t)}{\partial t} + \mathbf{v}\cdot\nabla u(\mathbf{x},t) = D\nabla^2 u(\mathbf{x},t) - ku(\mathbf{x},t), \tag{3}$$

  where: $\mathbf{v}$ is the velocity vector of the wind, D is the diffusion coefficient, k accounts for pollutant decay (e.g., due to chemical reactions or deposition) [Issakhov et al., 2020, Khan et al., 2013, Phillips et al., 2018].

- *Groundwater Pollution.* In aquifers, pollutants spread in three dimensions, but the movement is influenced by groundwater flow. The governing equation is:

  $$\frac{\partial u(\mathbf{x},t)}{\partial t} + \mathbf{v}\cdot\nabla u(\mathbf{x},t) = \nabla\cdot(D\nabla u(\mathbf{x},t)) - ku(\mathbf{x},t) + S(\mathbf{x},t), \tag{4}$$

  where: $\mathbf{v}$ is the groundwater velocity (advection term), D is the tensor of diffusion coefficients (anisotropic diffusion may occur in groundwater), k represents pollutant degradation, $S(\mathbf{x},t)$ is the external source of pollution [Banaei et al., 2021, Li et al., 2020, Prakash and Datta, 2014].

- *Soil Pollution with Bioremediation.* When modeling pollutant spread in soil, bioremediation (degradation by microorganisms) is often included. The reaction-diffusion equation becomes:

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = D\nabla^2 u(\mathbf{x},t) - k_1 u(\mathbf{x},t) - k_2 u^2(\mathbf{x},t), \tag{5}$$

  where: D is the diffusion coefficient in the soil, $k_1 u(\mathbf{x},t)$ accounts for first-order degradation (e.g., chemical decay), $k_2 u^2(\mathbf{x},t)$ describes a second-order degradation process, such as microbial consumption of the pollutant [Chen et al., 2024, Dhuldhaj et al., 2023, Raffa and Chiampo, 2021].

3 The Diffusion Model

Reaction-diffusion equations provide a flexible and powerful framework to model the spread of pollutants in diverse environments. By incorporating diffusion, advection, and reaction terms, these equations can capture the complex interplay of physical, chemical, and biological processes that govern the behavior of contaminants. Analytical solutions exist for simplified cases, but numerical methods are often required for more realistic scenarios. Diffusion models offer a foundational understanding of how pollutants spread and the factors driving this process, with key contributions from researchers who have explored the dynamics of pollution diffusion and the effectiveness of various mitigation strategies.

In our model, let us denote by $P(x,t)$ the pesticide level at a certain location x and time $t \in [0,T]$, with $x \in \Omega \subset \mathbb{R}^2$ a compact set and $T < +\infty$ the finite horizon. We assume that P is a C^1 function in time and C^2 in space, and it is integrable with respect to both variables, that is, $P \in C^{2,1}(\Omega \times (0,T)) \cap L^1(\Omega \times [0,T])$. Its diffusion equation is given by

$$\begin{cases} \dfrac{\partial P(x,t)}{\partial t} = \nabla_x \cdot (D_1(x)\nabla_x P(x,t)) - D_2(x)P(x,t) + (1-\theta(x,t))S(x,t), \quad \forall\ (x,t) \in \Omega \times (0,T], \\ \dfrac{\partial P(x,t)}{\partial n} = 0, \qquad \forall\ x \in \partial\Omega, \\ P(x,0) = P_0(x), \end{cases} \tag{6}$$

where $D_1 : \Omega \to \mathbb{R}^+$ is the diffusion coefficient of pesticides in various materials and such that $D_1(x) \geq d_1 > 0$, with d_1 a positive constant; $D_2 : \Omega \to \mathbb{R}^+$ is the natural decay rate for which there exist two constants $d_2, \tilde{d}_2 \in \mathbb{R}^+$ such that $d_2 \leq D_2(x) \leq \tilde{d}_2$, and $S : \Omega \times [0,T] \to \mathbb{R}^+$ models the exogenous source of pesticides at location x and at time t. At this stage, the term $\theta(x,t)$ is exogenous, and it describes the local effort to put in place at x and at the time t in order to limit the use of pesticides, where $\theta : \Omega \times [0,T] \to (0,1)$.
The term $(1-\theta(x,t))S(x,t)$ represents the amount of pesticide remaining at (x,t) after the effort's application and $P_0(x)$ is the initial distribution of pesticide level at place x. Such an initial distribution $P_0 : \Omega \to \mathbb{R}^+$ is a strictly positive function in $C^2(\Omega) \cap L^1(\Omega)$ where $C^2(\Omega)$ is the space of twice differentiable functions on Ω and $L^1(\Omega)$ is the set of all integrable functions over Ω. Finally, $\frac{\partial P}{\partial n}$ is the normal derivative of P at the boundary of Ω denoted by $\partial\Omega$. Under these hypotheses, the theory of parabolic equations ensures that the above boundary value problem (6) admits a unique classical solution [Lieberman, 1996]. Moreover, the strong maximum principle for parabolic equations guarantees that P is nonnegative for all $x \in \Omega$ and $t > 0$ [Protter and Weinberger, 2012].

Since $\theta \in (0,1)$, aggregating in space the diffusion pesticide dynamics (6), we get an upper and lower estimate for the spatial average pesticide level. The following result holds:

Theorem 1. *Suppose that* $\sup_{t\in[0,T]} \int_\Omega S(x,t)\,dx \leq M$ *for some positive* M*. Then, the spatial average pesticide level on* Ω *is such that*

$$e^{d_2 t}\int_\Omega P_0(x)\,dx \leq \int_\Omega P(x,t)\,dx \leq e^{\tilde{d}_2 t}\int_\Omega P_0(x)\,dx - \frac{M}{\tilde{d}_2}. \tag{7}$$

Proof. Aggregating in space the diffusion pesticide dynamic in (6), we get

$$\begin{aligned} \int_\Omega \frac{\partial P(x,t)}{\partial t}dx = &\int_\Omega \nabla_x D_1(x)\nabla_x P(x,t)\,dx + \int_\Omega D_1(x)\nabla_x^2 P(x,t)\,dx - \int_\Omega D_2(x)P(x,t)\,dx + \\ &\int_\Omega (1-\theta(x,t))S(x,t)\,dx. \end{aligned} \tag{8}$$

Since

$$\int_\Omega \nabla_x D_1(x)\nabla_x P(x,t)\,dx = D_1(x)\nabla_x P(x,t)\Big]_{\partial\Omega} - \int_\Omega D_1(x)\nabla_x^2 P(x,t)\,dx,$$

the Equation (8) becomes

$$\int_\Omega \frac{\partial P(x,t)}{\partial t}dx = -\int_\Omega D_2(x)P(x,t)\,dx + \int_\Omega S(x,t)\,dx - \int_\Omega \theta(x,t)S(x,t)\,dx. \tag{9}$$

Since $\theta(x,t) > 0$, by (9) follows that

$$\int_\Omega \frac{\partial P(x,t)}{\partial t}dx \leq -\,\tilde{d}_2 \int_\Omega P(x,t)\,dx + M. \tag{10}$$

Moreover, since $\theta(x,t) < 1$, by (9) follows that

$$\int_\Omega \frac{\partial P(x,t)}{\partial t}dx \geq -\,d_2 \int_\Omega P(x,t)\,dx. \tag{11}$$

Denoting by $\widetilde{P}(t) = \int_\Omega P(x,t)\,dx$ and applying Gronwall's inequality, by (10) and (11) one gets

$$e^{-d_2 t}\widetilde{P}(0) \;\leq\; \widetilde{P}(t) \;\leq\; e^{-\tilde{d}_2 t}\widetilde{P}(0) + \frac{M}{\tilde{d}_2},$$

and hence the thesis. □

4 The Optimal Control Problem

In this section, we formulate the policymaker's control problem aimed at reducing pesticide levels in the soil through strategic investments in organic agriculture as an alternative to conventional agricultural practices. This challenge is framed within a broader framework that seeks to balance social and economic considerations. The analytical formulation of the problem is the following:

$$\min_\theta J(P_0,\theta) := \int_0^T \int_\Omega e^{-\rho t}\left(\gamma(x,t)\,\theta^2(x,t) + c(x,t)P(x,t)\right)\,dx\,dt + \chi\, e^{-\rho T}\int_\Omega P(x,T)\,dx \tag{12}$$

subject to

$$\begin{cases} \dfrac{\partial P(x,t)}{\partial t} = \nabla_x \cdot (D_1(x)\nabla_x P(x,t)) - D_2(x)P(x,t) + (1-\theta(x,t))S(x,t), \quad \forall\ (x,t) \in \Omega\times(0,T], \\ \dfrac{\partial P(x,t)}{\partial n} = 0, \qquad \forall\ x \in \partial\Omega, \\ P(x,0) = P_0(x). \end{cases} \tag{13}$$

The objective function in (12) is composed of two distinct and interconnected terms, each reflecting a critical aspect of the policymaker's challenge. The first term represents the cost of effort associated with investing in organic agriculture. Specifically, this term quantifies the economic expenditure required to transition from conventional agricultural practices, which often rely on high levels of pesticide use, to organic methods that prioritize environmental sustainability. The cost per unit of effort in organic agriculture is captured by the function $\gamma : \Omega\times[0,T] \to \mathbb{R}^+$, which varies depending on the spatial domain Ω and the time interval $[0,T]$. This term emphasizes the financial burden of promoting organic practices, particularly in regions where the adoption of such methods may require significant infrastructural changes or educational outreach.

In addition to the direct costs of organic farming investments, this term also incorporates the social costs associated with maintaining a given level of pesticide contamination. The function $c : \Omega\times[0,T] \to \mathbb{R}_0^+$ denotes the social cost per unit of pesticide presence, which depends on the pesticide concentration P at a specific location x and time t. This social cost reflects the environmental and health impacts associated with pesticide use, including water contamination, ecosystem degradation, and risks to human health. By including this component, the first term accounts for both the immediate financial

implications of organic investments and the long-term societal benefits of reducing pesticide levels. The second term measures the total level of pesticides at the final horizon T with $\chi > 0$ a penalty to pay for the pesticide pollution that remains for future generations.
We address the problem of minimizing (12) subject to (13) on the functional space $C^{2,1}(\Omega \times (0,T)) \cap L^1(\Omega \times [0,T])$.

Definition 4.1. *A trajectory $[\theta(x,t), P(x,t)]$, with $P \in C^{2,1}(\Omega \times (0,T)) \cap L^1(\Omega \times [0,T])$ and θ piecewise $C^{2,1}(\Omega \times (0,T)) \cap L^1(\Omega \times [0,T])$, is admissible if P is a solution to problem* (13) *with control θ on $\Omega \times [0,T]$ and if the objective function* (12) *converges.*
A trajectory $[\theta^*(x,t), P^*(x,t)]$ for $t \in [0,T]$, $x \in \Omega$, is an optimal solution of problem (12) *subject to* (13) *if it is admissible and if it is optimal in the set of admissible trajectories; that is, for any other admissible trajectory $[\theta(x,t), P(x,t)]$, the value of the integral* (12) *is not lower than its value corresponding to $[\theta^*(x,t), P^*(x,t)]$.*

Using Pontryagin's Maximum Principle, we derive the optimality conditions for (12)-(13). We define the Hamiltonian function:

$$\begin{aligned} H(P,\lambda,\theta,x,t) = &\gamma(x,t)\,\theta^2(x,t) + c(x,t)P(x,t) + \\ &\lambda(x,t)\left[\nabla_x \cdot (D_1(x)\nabla_x P(x,t)) - D_2(x)P(x,t) + (1-\theta(x,t))S(x,t)\right], \end{aligned}$$

where $\lambda(x,t) \in C^{2,1}(\Omega \times (0,T)) \cap L(\Omega \times [0,T])$ is the costate variable. The optimality conditions are defined as:

- Stationary condition:
$$\frac{\partial H}{\partial \theta} = 2\gamma(x,t)\theta(x,t) - \lambda(x,t)S(x,t) = 0$$
- Costate equation:
$$-\frac{\partial \lambda(x,t)}{\partial t} = -(D_2(x)+\rho)\lambda(x,t) + c(x,t) + \nabla_x D_1(x)\nabla_x\lambda(x,t) + D_1(x)\nabla_x^2\lambda(x,t). \tag{14}$$
- State equation:
$$\frac{\partial P(x,t)}{\partial t} = \nabla_x \cdot (D_1(x)\nabla_x P(x,t)) - D_2(x)P(x,t) + (1-\theta(x,t))S(x,t).$$
- Transversality condition:
$$\lambda(x,T) = \chi$$
- Neumann boundary condition:
$$\frac{\partial P(x,t)}{\partial n} = 0, \qquad \frac{\partial \lambda(x,t)}{\partial n} = 0, \qquad \text{for } x \in \partial\Omega$$
- Initial condition:
$$P(x,0) = P_0(x), \quad \text{for } x \in \Omega$$

The optimal control $\theta^*(x,t)$ can be obtained by solving the stationary condition for θ, which gives:

$$\theta^*(x,t) = \frac{\lambda(x,t)S(x,t)}{2\gamma(x,t)}. \tag{15}$$

Proposition 1. *If the social cost $c(x,t)$ is space independent, the natural decay rate is constant, namely $D_2(x) = D_2$, and θ is piecewise $C^{2,1}(\Omega \times (0,T)) \cap L^1(\Omega \times [0,T])$ then there exists a spatially homogeneous solution for the costate variable, namely*

$$\lambda(x,t) = e^{(D_2+\rho)t}\left[\chi e^{-(D_2+\rho)T} + \int_t^T c(s)\, e^{-(D_2+\rho)s}\, ds\right]. \tag{16}$$

In this case, the optimal effort is provided by

$$\theta^*(x,t) = \frac{e^{(D_2+\rho)t}}{2\gamma(x,t)}\left[\chi e^{-(D_2+\rho)T} + \int_t^T c(s)\, e^{-(D_2+\rho)s}\, ds\right] S(x,t).$$

Proof. Let us prove that the function $\lambda(x,t) = \lambda(t)$ solves the costate equation (14). Substituting for $\lambda(t)$ and applying the above assumptions, we obtain that

$$\frac{\partial \lambda(t)}{\partial t} - (D_2+\rho)\lambda(t) + c(t) = 0, \qquad \lambda(T) = \chi,$$

whose solution is

$$\lambda(t) = e^{(D_2+\rho)t}\left[\chi e^{-(D_2+\rho)T} + \int_t^T c(s)\, e^{-(D_2+\rho)s}\, ds\right]$$

□

Remark 1. *Note that if $c(x,t) = c$ and $\gamma(x,t) = \gamma$, i.e., they are both constant for every $(x,t) \in \Omega \times [0,T]$, by Proposition 1 it follows that*

$$\lambda(t) = \frac{e^{(D_2+\rho)(t-T)}\left(\chi(D_2+\rho) - c\right) + c}{D_2+\rho},$$

and

$$\theta^*(x,t) = \left[\frac{e^{(D_2+\rho)(t-T)}\left(\chi(D_2+\rho) - c\right) + c}{2\gamma\,(D_2+\rho)}\right] S(x,t). \tag{17}$$

Moreover, if there exists $L > 0$ such that $S(x,t) \le L$ for every $(x,t) \in \Omega \times [0,T]$, $\chi(D_2+\rho) > c$ and $\chi L < 2\gamma$ then

$$0 < \theta(x,t) < 1.$$

The following example 1 illustrates the behavior of the effort θ and the corresponding pesticide level P on the final horizon T for two different social costs c. Note that when $t = T$, the expression of θ in (17) is independent of c, so we report only one graph for θ.

Example 1. *We set $\Omega = [0,3] \times [0,3]$, and let (a,b) represent the coordinate variables on Ω. We also set $T = 5$, $D_1 = 0.00016$, $D_2 = 0.77$, $\rho = 0.01$ and consider $S(a,b,t) = 0.4(a+b+0.5t+1)$ so that $\chi = 1$ and $\gamma = 2$. We also fix the initial condition $P_0(a,b) = 4$, for every $(a,b) \in \Omega$. We generate the graph of both θ and P for $c = 0.05$ and $c = 0.75$, respectively.*

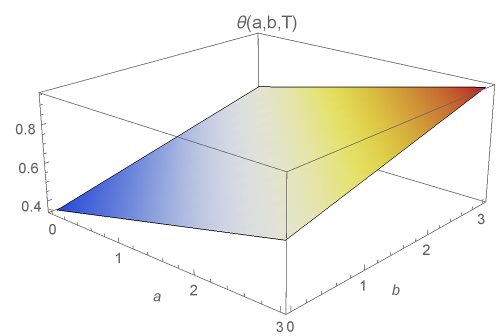


Figure 1: The optimal effort θ for different locations in Ω

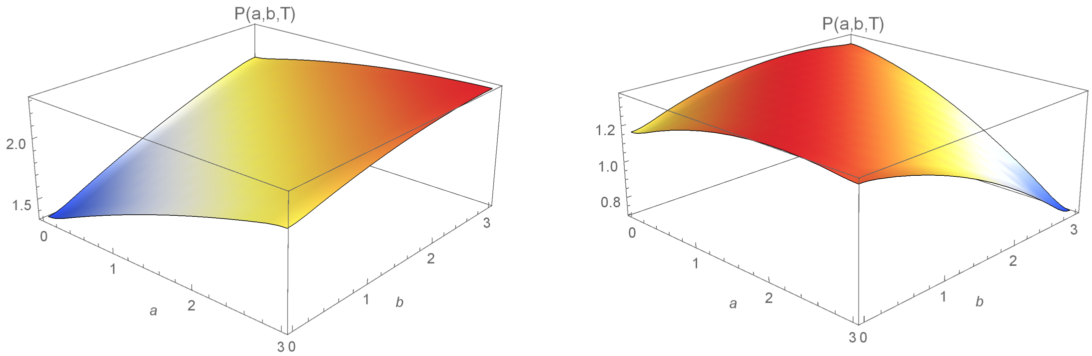


Figure 2: The pesticide level $P(x, t)$ for $c = 0.05$ (left) and for $c = 0.75$ (right).

The numerical example reveals a clear link between the social cost of pesticide exposure and its spatial concentration. Specifically, increasing the social cost leads to a significant reduction in pesticide levels across the spatial domain, reflecting the policymaker's goal of balancing the costs of pesticide exposure and the effort required for transitioning to organic agriculture. Higher social costs incentivize stronger efforts to reduce pesticide levels, especially in areas with higher contamination. This results in a more uniform distribution of the effort and a corresponding reduction in pesticide concentration. The interplay between diffusion and optimal effort allocation ensures that localized hotspots of contamination are minimized. These findings suggest that raising awareness of pesticide-related social costs or implementing stricter regulations can encourage more effective policies, targeting regions of high contamination and achieving substantial social benefits.

The model incorporates diminishing returns in the effectiveness of effort, meaning that as more effort is applied in a given region, the additional reduction in pesticide concentration becomes less significant. This encourages a balanced spatial allocation of effort, particularly when the social cost of pesticide exposure is high, ensuring that all regions experience meaningful reductions in pesticide levels.

While the results focus on the spatial domain, the temporal dimension also plays a role. Over time, the diffusion process redistributes pesticide concentrations, and the higher social cost influences the policymaker to act proactively by applying effort earlier in the planning horizon. This leads to a more substantial cumulative reduction in pesticide concentration by the end of the simulation period.

5 Dataset Description

In this section, we describe the database used to test the validity of our theoretical model presented in sections 3 and 4. It contains measurements of atrazine concentration in French groundwater between 2016 and 2023 taken at 675 water extraction sites in Metropolitan France, excluding Corsica. The reason behind the exclusion of Corsica lies in the fact that the location is crucial for understanding the spread of pesticides. Therefore, French groundwater locations that are not geographically connected and cannot influence each others' pesticide levels are not important for our purposes.
This information was retrieved from a publicly available dataset created by "Le Monde", a leading French daily newspaper, using data from the groundwater data access portal (`https://ades.eaufrance.fr`).

In this paper, we focused exclusively on atrazine measurements for several reasons. First, atrazine is one of the most widely used herbicides in developed countries and one of the most frequently detected in groundwater. In the US alone, its use incurs approximately $12 billion annually in environmental and healthcare costs [Pimentel et al., 2005]. Although the European Union banned atrazine in 2004 248 [2004], residual levels from past applications continue to pose concerns. Atrazine entered the environment in manifold ways: through its historic application in fields, crops, highways and railroads, and to a lesser extent during manufacturing, transport, and disposal. Remobilization and leaching allowed it to pollute groundwater, where its persistence extended its presence in the environment as well as its effects on human beings due to exposure [Vonberg et al., 2014]. Research by Jablonowski et al. [2009] demonstrates that in Germany, where atrazine was banned in 1991, it remains detectable in the groundwater 22 years later. Our data reflects an alarming persistence of atrazine in France groundwater as well. After the ban, ideal legal limit of atrazine detectable in groundwater should be null. However, under the Drinking Water Directive 83 [1998] and Groundwater Directive 118 [2006], the concentration of the substance cannot exceeded safety threshold level of 0.1µg/L. This happened in 12 different measurement sites and a total of 96 times in the years considered. Furthermore, it exceeded the concentration of 0.01µg/L - which is the minimum atrazine concentration in drinkable water that has relevant exposing effects for humans [Harper et al., 2020] - in 600 different locations and 3871 times. The long-term presence and the effects of long-lasting environmental exposure to the substance are not completely known, and therefore, concerning. Note that these data are solely related to the parent pesticide. Its degradation products or metabolites, which represent potential hazards for health and the environment in different ways, have not been considered. Secondly, atrazine is linked to a serious health issue with growing socio-economic impact and scientific importance in recent years: infertility. While the connection between certain pesticides and cancer has been thoroughly studied and documented, research on their effects on fertility still presents some gaps. Fertility is a crucial issue for developed countries today, as its levels have significantly decreased over the past decades, undermining societal long-term sustainability and economic growth. In a recent work, Levine et al. [2023] confirmed a significant decline in sperm count from the 1970s, that continued to become steeper since the beginning of this century. The decline is recognized as a global public health crisis that must be addressed by researching chemical exposures, including pesticides, especially due to their trans-generational implications. Infertility significantly impacts developed countries' economies and pension systems, especially in those with fertility rates below the replacement level of approximately 2.1 children per woman, like Germany, Italy, and France (with 1.8 rate in 2022) [OECD, 2024, Doepke et al., 2022]. The economic threat to pension systems is twofold: (1) a shrinking working-age population reduces the tax base, limiting funds for pensions and social security, and (2) an increasing old-age dependency ratio strains pay-as-you-go pension systems, as fewer workers support more retirees. In the discussion on pesticide hazards, researchers such as Giulioni et al. [2022], Fucic et al. [2021], and Moreira et al. [2021] have emphasized the importance of infertility research. They suggest that more attention should be given to this area because of its emerging, long-term public health significance, the lack of studies, and fewer funding compared to cancer, which has a more established research base. Atrazine toxicity has been thoroughly studied in Jowa and Howd [2011], Gammon et al. [2005], Jablonowski et al. [2011]. Although its carcinogenic potential remains controversial, major regulatory agencies, including the International Agency for Research on Cancer (IARC) and the United States Environmental Protection Agency (EPA), have classified atrazine as unlikely to be carcinogenic to humans [Simpkins et al., 2011]. However, atrazine exposure is associated with other significant health effects, including DNA strand breaks, hormonal imbalances, and reproductive system alterations [Agency for Toxic Substances and Disease Registry (US), 2003]. Human reproductive risk associated with atrazine exposure was discussed in the seminal work of Swan et al. [2003], which reduced sperm concentration and mobility in fertile men environmentally exposed to atrazine. Additionally, Cragin et al. [2011] found that women exposed to atrazine through drinking water exhibited increased menstrual cycle irregularities, prolonged follicular phases, and reduced levels of endocrine biomarkers associated with ovulatory infertility. Although interest in human studies on atrazine-related infertility is growing, the body of evidence remains limited compared to animal studies, which consistently demonstrate adverse effects on male reproductive health, particularly sperm quality and quantity, critical factors for fertility. Laboratory tests on animals, including rats and fish, demonstrate observable effects on fertility [Bautista et al., 2018, Harper et al., 2020]. These effects occur at various exposure levels, and involve mechanisms such as endocrine disruption, oxidative stress, and changes in gene expression. This disparity between human and animal research highlights a critical gap in the scientific literature. While animal models indicate substantial reproductive risks, human studies are constrained by limited scope and data. The last reason leading us to focus on atrazine is the number of observations available in the original dataset. This is one of the most frequently detected pesticides in water extraction points across the studied region of France. Notably, it was found in groundwater more often than other non-banned pesticides, such as metolachlor, a widely used pesticide in France with similar leaching potential, providing sufficient observations to validate our model.

Due to technical reasons related to the model's discretization and the regression method used to estimate its parameters, we proceeded by obtaining a balanced panel dataset over all the years of the time period considered. In particular, the discretization of the model forces the observations to be measured at the same time intervals. However, since the exact dates of the measurements vary significantly, we averaged all the measurements related to a single year into one figure. Since some measurements of water extraction points were missing for one or multiple years, we finally considered only water extraction site with at least one observation per year. Figure 3 illustrates the locations of selected groundwater points. Most are concentrated in the northern part of the country, around Paris, with some clusters also present in the southern regions. This does not surprise, as the areas with high concentration of locations are those where crop production is the highest: Paris Basin, South-West and the upper part of the Rhône Valley [Donfouet et al., 2017].

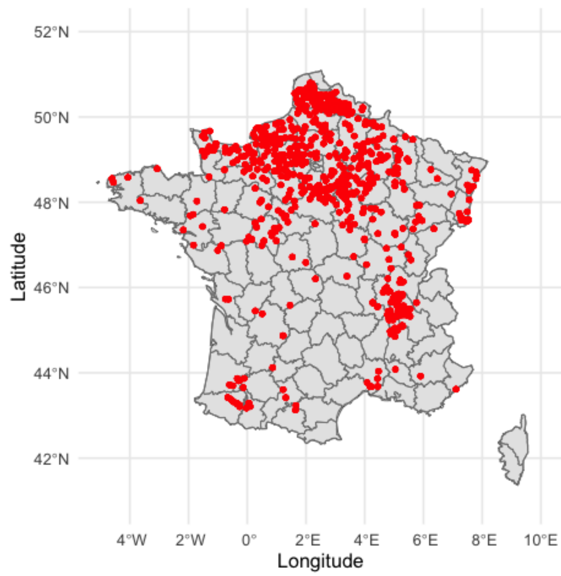


Figure 3: Location of groundwater points in Metropolitan France

The final dataset consists of a total of 5400 measurements, one per each considered year for all 675 locations. The measured atrazine values have a mean of 0.02347µg/L, ranging from a minimum of 0.002µg/L to a maximum of 0.3975µg/L. The distribution of atrazine levels is represented in Figure 4.

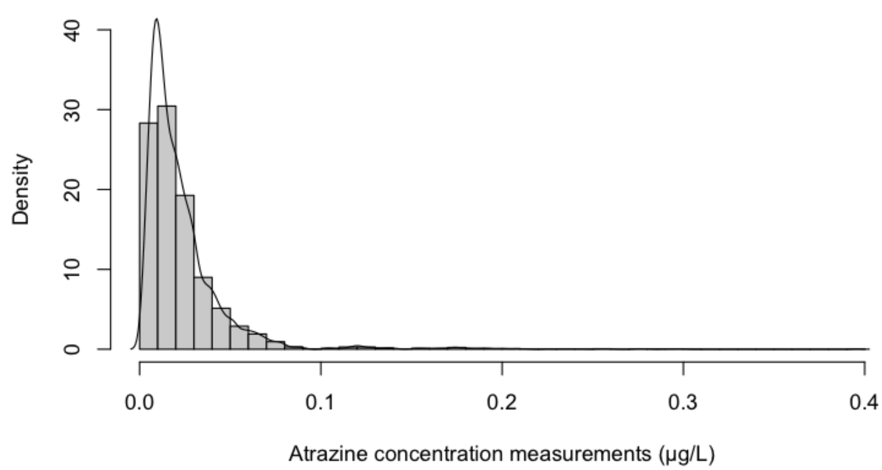


Figure 4: Distribution of atrazine concentration measurements

The descriptive statistics related to annual measurements of atrazine concentration are summarized in Table 1. It is noteworthy that the average atrazine concentration in France's groundwater, after a slight increase in 2017, decreased from 0.02828µg/L in 2016 to 0.01940µg/L in 2023. Concurrently, the standard deviation decreased from 0.02920 to 0.02190 indicating reduced variability of atrazine concentration over time (see Figure 5). This output is consistent with expectations of a decreasing concentration of atrazine in groundwater over time following EU ban. However, the decrease is more pronounced in the maximum values, while the decrease in minimum levels is less significant in magnitude. It should be noted that the average concentration of atrazine is above 0.01µg/L, the lower limit of atrazine concentration for drinking water mentioned earlier. In fact, 71.69% of measurements show concentrations above this level. However, the concentration exceeds the legal threshold in only 1.78% of measurements. Despite the ban, atrazine concentrations in groundwater frequently remain at levels that could pose health risks if people are chronically exposed.

Year	**Mean**	**Median**	**Min**	**Max**	**SD**	**N**
2016	0.02828	0.02100	0.00300	0.29580	0.02920	675
2017	0.02957	0.02125	0.00325	0.39575	0.03207	675
2018	0.02394	0.01771	0.00200	0.26000	0.02518	675
2019	0.02226	0.01600	0.00200	0.24400	0.02333	675
2020	0.02182	0.01600	0.00200	0.27680	0.02355	675
2021	0.02185	0.01600	0.00200	0.30025	0.02391	675
2022	0.02060	0.01460	0.00200	0.25240	0.02221	675
2023	0.01940	0.01335	0.00200	0.23800	0.02190	675

Table 1: Yearly descriptive statistics of atrazine concentration (µg/L)

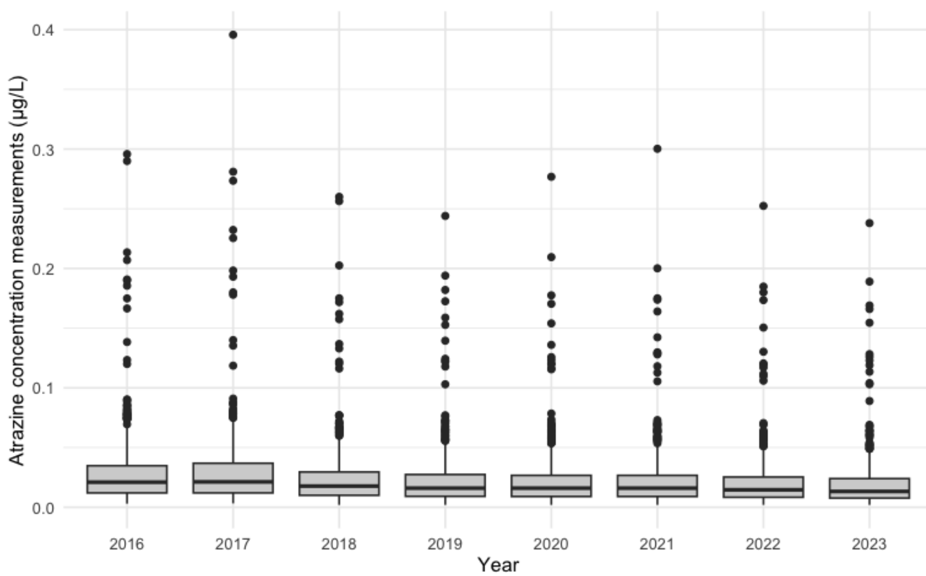


Figure 5: Density of Atrazine concentration measurements

Pesticide pollution is not confined to the areas where pesticides are applied. Once released into the environment, these chemicals can migrate through soil and water, contaminating nearby regions and groundwater. To model the environmental diffusion of atrazine we use the groundwater ubiquity score (GUS) index, introduced by Gustafson [1989] as an indication of pesticides' potential leaching properties in the environment. The author introduced the index specifically for assessing the leachability of pesticides in groundwater by considering the properties of the pesticides only. This is perfectly in line with our purposes as it is going to represent the variable assessing the spread of the pesticides. This index is based on two other measures: the soil sorption constant and the half-life.
The soil sorption constant (i.e., K_{OC}) was originally proposed by Hamaker [1975], but McCall et al. [1980] demonstrated the correlation between the K_{OC} and the movement of a chemical through the soil. In fact, this constant expresses technically the spreading properties of the substance or its partition coefficient between soil and water [Swann et al., 1983]. K_{OC} can be considered a substance-specific,

soil-independent metric that describes the fate of pesticides in the environment. However, the actual movement of pesticides in the soil is related to numerous variables other than substance-specific ones. They are mainly related to the type of soil used and meteorology. The half-life, conventionally represented by the variable $t_{1/2}$, is another variable that describes the persistence of the chemical in the soil. In particular, it is the time the pesticide takes to reach half of its presence in the environment through degradation, and it is expressed in days [Salvia et al., 2018]. This process is led by the interaction between pesticides and several agents present in the environment, which could be physical, chemical, or biological. For example, the photolysis of the sunlight, the oxidation and other reactions with different chemicals or the hydrolysis in water [Kumar et al., 2018, A. et al., 2022]. Accordingly, the half-life can be computed both in soil and in water. Gustafson [1989] considered only the half-life in the soil for computing the index. This is to better understand how the pesticides, once normally applied to the fields, persist into the soil and potentially reach surrounding groundwater.
Even if broadly accepted, the use of K_{OC} only as a proxy for chemical mobility in the environment must be cautiously considered. Its complete ability to describe the geographical fate of pesticides has been criticized (see, e.g., Jarvis [2016] or von Oepen et al. [1991]). However, it is meaningful in modeling and universally used to compare the mobility of different pesticides [Wauchope et al., 2002]. The same concerns hold for the half-life variable since pesticides could dissipate according to the extent of the interaction between the substance and the mentioned degradation processes [Shen et al., 2022]. Taking both variables into consideration is an additional step for granting the goodness of our pesticides' mobility proxy. Although still regarded as a relatively simplistic method to assess chemical transport in the environment, the GUS is seen as an effective index of chemical mobility. Despite its limitations, it is one of the most widely used indices for this type of metric, and several other indexes directly depend on it [Pawlowski et al., 2023]. The Gus index is computed as follows:

$$\text{GUS} = log_{10}(t_{1/2}^{\text{soil}}) \times [4 - log_{10}(\text{K}_{OC})],$$

where $t_{1/2}^{\text{soil}}$ is the half-life of the pesticide in the soil and K_{OC} the soil sorption constant.

We consider the GUS index of atrazine, as well as the ones of the other pesticides considered, to weight the impact of atrazine on the social costs related to the use of pesticides; further details below, from the pioneering paper of Gustafson [1989].
In our theoretical framework, the social costs of pesticide use encompass all costs associated with exposure to these chemicals, including environmental pollution and health-related impacts. Such data are often limited due to measurement challenges and their sensitive nature. To quantify these costs for the selected pesticide, we use the cost of pesticide removal from groundwater in Metropolitan France as a proxy. This government-borne cost reduces citizens' exposure to pesticides in drinking water, thereby potentially decreasing health-related social costs by lowering the incidence of associated illnesses. According to a 2011 report by France's General Commission for Sustainable Development [Bommelaer and Devaux, 2011], the estimated cost for the pesticide-related water treatments in France amounts to 32 to 105 billion euros. As the source did not provide any additional information regarding the distribution, we are going to use the average of these two bounds (68.5 billion euros). These figures are the country-wise estimates of the treatment costs to reduce the excessive concentration of pesticides in the water. The fact that there is no unique large-scale cleaning method does not allow for higher precision. In the report, the above cost is necessary to treat 24.7% of the 2,000 billion m^3 total groundwater stock. The treatment would eliminate 526 tonnes of pesticides in the treated water. This means that 68.5 billion euros allow for a decrease of 1.06 µg/L in pesticide concentration in almost a quarter of France's groundwater stock. If we normalize this, as the groundwater stock does not change and if the relationship between costs and pesticide concentration reduction is linear, we obtain the cost of reducing the concentration of France's groundwater by 0.1 µg/L, that is 6.46 billion of euros. If we divide this by the treated amount of groundwater (27% of 2,000 billion m^3), we can obtain the estimate of the cost per liter of groundwater to reduce the pesticide concentration by 0.1 µg/L, that is ≈ 0.00001308 euro/L.
The cost of removing pesticides from groundwater is weighted according to the pesticide's GUS index against that of the other 28 pesticides studied by Gustafson [1989]. The average of the considered GUS indexes is 1,553. We notice that Atrazine leaches and spreads in the groundwater more than the average considered pesticides. We conclude that its presence is going to be spread in a larger amount of groundwater with respect to the average, and so the price of treating water from Atrazine must be

higher. Scaling the estimated cost of reducing the concentration of French groundwater by 0.1 µg/L according to Atrazine's GUS index of 3,68 gives us the final cost of reducing Atrazine's presence in French groundwater by 0.1 µg/L, that is ≈ 0.00004408 euro/L. The cost of water treatment for removing pesticides was provided by the French General Directorate of Sustainable Development (Commissariat général au dèveloppement durable, or CGDD) in the 2011 report on the costs of the main agricultural water pollution Bommelaer and Devaux [2011]. Finally, to assess the difference between organic and conventional agriculture we focused on the difference in profitability between the two farming methods. In particular, this can be seen as the opportunity cost of picking one farming method with respect to the other, and vice versa. The considered indicator is computed by taking the ratio of the gross operating profit of the organic and conventional farming methods per unit of output. To obtain such information, data on different farming sectors' profits were obtained and then weighted according to the distribution of the workforce within the two production methods. By doing so, we obtained the average cost of the two agriculture methods, and their relationship gave us the opportunity cost of selecting organic over conventional agriculture. This value is equal to 1.6327. These data, which date back to 2020, are available in Devauvre [2024]. The goodness of the data is also corrected for the presence of subsidies, which could affect the operating profits of the two different methods. The author specifies that the weight of government support in the composition of the operating surplus of both conventional and organic agriculture is basically equivalent (44.6% and 44.4%, respectively).

6 Model Discretization and Econometric Estimation

This section aims to estimate the unknown parameters of the diffusion model described in (6) using the data presented earlier. To achieve this, we first discretize the diffusion equation through finite differences. Next, we estimate the Laplacian as the quadratic surface in (18) using the Geographically Weighted Regression approach. Finally, we estimate D_1 and D_2, along with the source function S and the effort θ.

6.1 From Theory to Empirics

We consider the generalized diffusion equation in which the coefficients D_1 and D_2 are constant. To keep things simple and avoid overly complex notation, in the sequel we will denote by a and b the two spatial components of the vector $x \in \Omega$. Then, we have:

$$\frac{\partial P(a,b,t)}{\partial t} = D_1 \nabla^2 P(a,b,t) - D_2 P(a,b,t) + (1 - \theta(a,b,t)) S(a,b,t),$$

where:

- $P(a,b,t)$: Observed concentration at the location (a,b) and time t;
- $D_1 > 0$: Diffusion coefficient (to be estimated);
- $\nabla^2 P(a,b,t)$: Laplacian of $P(a,b,t)$, representing the spatial second derivatives at the location (a,b) and time t;;
- $D_2 > 0$: Decay rate (to be estimated);
- $S(a,b,t)$: Source term at the location (a,b) and time t;
- $\theta(a,b,t)$: Effort at the location (a,b) and time t.

To build the econometric model, we discretize the diffusion equation. Given a point (a_i, b_j) on the grid, and using the finite differences method, we get:

1. The temporal derivative:

$$\frac{\partial P(a_i,b_j,t_k)}{\partial t} \approx \frac{P(a_i,b_j,t_{k+1}) - P(a_i,b_j,t_k)}{t_{k+1} - t_k};$$

2. The Laplacian in two dimensions:

$$\nabla^2 P(a_i, b_j, t_k) \approx \frac{P(a_{i+1}, b_j, t_k) - 2P(a_i, b_j, t_k) + P(a_{i-1}, b_j, t_k)}{\Delta a^2} + \frac{P(a_i, b_{j+1}, t_k) - 2P(a_i, b_j, t_k) + P(a_i, b_{j-1}, t_k)}{\Delta b^2},$$

where Δa and Δb are the spatial grid steps that are supposed to be constant (independent from i and j). If the spatial grid is not uniform, we can proceed in the following way: for a fixed t_k, around a point (a_i, b_j), consider the neighbouring points within a certain radius r and then fit a quadratic surface

$$\beta_0 + \beta_1 a_i + \beta_2 b_j + \beta_3 a_i^2 + \beta_4 a_i b_j + \beta_5 b_j^2, \tag{18}$$

where the coefficients $\beta_3, \beta_4, \beta_5$ correspond to the second-order terms. All coefficients, β_0, β_1, $\beta_2, \beta_3, \beta_4, \beta_5$, can be estimated using the weighted least square method, and using the points in the circle of radius r (here we assume that the weights are $e^{-d_{ij}^2}$ where d_{ij} is the distance in km from the central point (a_i, b_j) and the neighbouring points). The Laplacian at (a_i, b_j) is:

$$\nabla^2 P(a_i, b_j, t_k) = 2\beta_3 + 2\beta_5.$$

Rearranging the discretized terms to isolate D_1 and D_2, we get the following equation:

$$P(a_i, b_j, t_{k+1}) - P(a_i, b_j, t_k) = (t_{k+1} - t_k) \times \left[D_1 \nabla^2 P(a_i, b_j, t_k) - D_2 P(a_i, b_j, t_k) + (1 - \theta(a_i, b_j, t_k)) S(a_i, b_j, t_k)\right], \tag{19}$$

which provides the basis for the regression model. The dependent variable is the first difference of pesticide level $\Delta P \equiv P(a_i, b_j, t_{k+1}) - P(a_i, b_j, t_k)$, and the independent variables are 1) the computed Laplacian $\nabla^2 P(a_i, b_j, t_k)$, 2) the pesticide level at time t_k, $P(a_i, b_j, t_k)$ and 3) source and effort terms, $S(a_i, b_j, t_k)$ and $\theta(a_i, b_j, t_k)$, respectively.

6.2 Estimation of the Laplacian using Geographically Weighted Regression (GWR)

Addressing the persistence of pesticides in groundwater is a complex task as the elements that can affect the process are numerous [Huggins et al., 2023]. Given that groundwater is an interconnected system and atrazine is a pesticide that leaches well, understanding how its presence in one location influences surrounding areas is crucial for efficient water treatment and reducing health costs related to pesticide exposure.
Through the data collected, we estimate the theoretical model diffusion and decay parameters, D_1 and D_2, and finally compute the source term and the effort, S and θ. We first estimate the coefficients β_k of (18) by using the Geographically Weighted Regression (GWR henceforth). GWR was developed by Brunsdon et al. [1996] to overcome the limitations of global regression models, which do not adequately address local variations. The basic principle of GWR consists of estimating local models using least squares, with each observation being weighted by a decreasing function of its distance to the estimation point. GWR belongs to the family of variable coefficients models, where the regression coefficients are not fixed but depend on the geographical coordinates of observations:

$$y_{ij} = \sum_k \beta_k(a_i, b_j) x_{ijk} + \varepsilon_{ij}, \tag{20}$$

where $y_{ij} \equiv \nabla^2 P(a_i, b_j, t_k)$ is the Laplacian, (a_i, b_j) are geographical coordinates of points, $\beta_k(a_i, b_j)$ are the local coefficients to estimate and x_{ijk} the corresponding independent variables. Finally, ε_{ij} is the error term.

The estimation of coefficients is based on Tobler's law: 'Everything is related to everything else, but near things are more related than distant things'. In practice, this means that the closer the two observations are geographically, the more similar the influence of the explanatory variables on the dependent variable. In other words, the coefficients of the explanatory parameters in the regression are closer to each other. We can express the GWR estimator (in the case of a cross-sectional dataset) as:

$$\hat{\beta}(a_i, b_j) = [X^T W(a_i, b_j) X]^{-1} X^T W(a_i, b_j) Y, \tag{21}$$

where $\hat{\beta}(a_i, b_j)$ is a $k \times 1$ matrix of estimated parameters at (a_i, b_j), X is a $n \times k$ matrix of features, $W(a_i, b_j)$ is a $n \times n$ matrix of weights and Y is a $n \times 1$ vector. The main choice of the researchers when using GWR concerns $W(a_i, b_j)$, the spatial weight matrix between points determined by a kernel function. The three key parameters to determine are 1) the shape of the kernel, 2) a fixed or adaptive kernel and 3) the bandwidth (radius).

For determining the three key parameters mentioned above, we decided to use an empirical approach. For the shape of the kernel , we chose between shapes that, in principle, allow all observations to be weighted: the Gaussian and the exponential. These seemed more appropriate than non-continuous functions with compact support, such as bi-square or tricube, as leaching does not necessarily stop at a predefined threshold. Between the two options, we preferred the Gaussian due to the higher R^2 value obtained (See Table A1 in the Appendix). Additionally, the Gaussian distribution is the most widely used empirically.

We opted for a fixed kernel because the leachability of atrazine is constant and described by its GUS index. Unlike many empirical applications of GWR that focus on socio-economic variables — where an adaptive kernel is appropriate to address spatial density heterogeneity — our case differs significantly. Instead, the bandwidth is selected using a pure Data Generating Process (DGP) approach that involves selecting the radius that maximize the goodness of fit. As shown in Figure A1 in the Appendix, the optimal bandwidth corresponds to a 20 km radius. Finally, to address the sensitivity of Ordinary Least Squares (OLS)-based methods to outliers, we implement a robust GWR algorithm that reduces the impact of outliers on parameter estimates. Unlike basic GWR, the robust version handles local outliers by using an M-estimator with a robust loss function. Robust GWR implements an Iteratively Reweighted Least Squares (IRLS) algorithm to calculate the regression coefficients. In each iteration, it calculates the residual errors, assigns robust weights to the errors based on the loss function, and then updates the local regression coefficients until convergence. Specifically, a Huber function is used to reduce the impact of outliers (i.e., those with residual errors greater than two standard deviations, which constitute 2.67% of the total) on the model estimation. By using this function, observations with smaller residuals are downweighted according to a quadratic loss, while outliers are downweighted using a linear loss function. The spatial weights (based on the kernel and distance matrix) are combined with the robust weights to produce local estimates that are robust to outliers.

As we deal with panel data and not cross-sections, we create a loop to perform GWR every year. It allows us to obtain β_k coefficients for each location and every year. We then use $\hat{\beta}_3$ and $\hat{\beta}_5$ to estimate the Laplacian and finally carry out the estimation of the diffusion model.

6.3 Estimation of the diffusion model

Given that in our data $t_{k+1} - t_k = 1$ and by rewriting any generic t_k with t, we can simplify the theoretical diffusion model (19) as:

$$\Delta P = D_1 \cdot \nabla^2 P(a_i, b_j, t) - D_2 P(a_i, b_j, t) + (1 - \theta(a_i, b_j, t)) S(a_i, b_j, t).$$

where $\Delta P \equiv P(a_i, b_j, t+1) - P(a_i, b_j, t)$. Since we do not observe $\theta(a_i, b_j, t)$ and $S(a_i, b_j, t)$, we approximate them using the panel structure of our data. More specifically, we set the following empirical diffusion model:

$$\Delta P = D_1 \cdot \nabla^2 P(a_i, b_j, t) - D_2 P(a_i, b_j, t) + \mu_{ij} + \mu(t) + \epsilon_{ijt},$$

where μ_{ij} represents the location-specific fixed effects, $\mu(t)$ represents a temporal effect that can be either fixed (time fixed effects) or time-varying (trend) and ϵ_{ijt} is the error term. In other words, we assume that $(1 - \theta(a_i, b_j, t)) S(a_i, b_j, t) = \mu_{ij} + \mu(t) + \epsilon_{ijt}$. The choice for the modelisation of $\mu(t)$ will be based on a DGP approach as no theoretical arguments allows us to prefer a priori a trend or time fixed effects. We thus compare goodness of fit of a two-way fixed effect model (assuming $\mu(t) = \sum_t \eta_t t$, with η_t the temporal fixed effects) with the one of a one-way fixed effect model with a linear trend (assuming $\mu(t) = \varphi t$, an homogeneous trend).

	ΔP	ΔP
$\nabla^2 P$	0.00016^{***}	0.00012^{***}
	(0.00002)	(0.00002)
P	0.77018^{***}	0.76192^{***}
	(0.04013)	(0.0145)
t	-0.00101^{***}	-
	(0.00007)	
Num. obs.	4,725	4725
R^2	0.4097	0.4069
Adjusted R^2	0.3109	0.3068
Individual FE	Yes	Yes
Time FE	No	Yes
F Statistic	184.828^{***}	210.448^{***}
Note:	*p<0.1; **p<0.05; ***p<0.01	

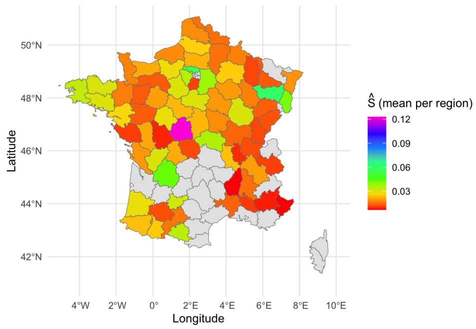
Table 2: Diffusion model outputs: individual effect vs two-way effects

Table 2 presents the model estimates of the coefficients, with their robust standard errors in parenthesis. We observe that the one-way fixed-effect model with linear trend provides a slightly better fit, as the R^2 is higher. This indicates that modeling the time effect as a linear trend better explained the observed dynamics of pollution. Therefore, we consider the model's estimates in Column 1 as our preferred specification. To control for heteroskedasticity, all estimations use robust standard errors. As can be seen in Table 2, the two key parameters of our diffusion model have the expected sign and are strongly statistically significant. In our preferred specification, we estimate the diffusion coefficient D_1 as 0.00016, highlighting significant leaching of atrazine in the groundwater system. Our results also show the natural decline of this pesticide concentration over time as the decay coefficient D_2 is estimated at 0.77018. The estimated values of these two key parameters are robust to changes in the way we introduce a temporal effect. In fact, the coefficients D_1 and D_2 are relatively stable whether we use time trend or time-fixed effects. Finally, the coefficient of the time variable, φ, is equal to -0.00101 and represents a decrease of ΔP over time. From the preferred specification, we collected estimates for the individual effects $\hat{\mu}_{ij}$ (see Figure A2), temporal effects $\hat{\varphi}t$ and the error terms $\hat{\epsilon}_{ijt}$ (see Figure A3).

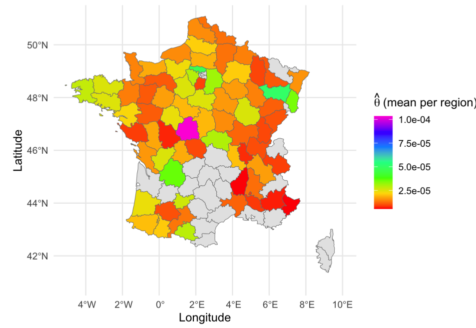
As previously mentioned, the sum of these three elements allows us to compute the estimated values of $S(a_i, b_j, t)$ and $\theta(a_i, b_j, t)$, involved in the last part of our diffusion model. More specifically, we first compute $\hat{S}(a_i, b_j, t)$ by substituting the expression of $\theta(a_i, b_j, t)$, as provided in Remark 1, into $(1 - \theta(a_i, b_j, t))S(a_i, b_j, t)$, and then solve the resulting quadratic equation for $S(a_i, b_j, t)$. Being quadratic, the equation generates two solutions for the source level. We assume the lowest value of the source to be the one that generates the observed pollution levels. Consequently, among the two solutions, we keep the one yielding the lowest values of $\hat{S}(a_i, b_j, t)$, and then substitute this into expression (17) to finally obtain the effort $\hat{\theta}(a_i, b_j, t)$.

The maps of France in Figure 6 illustrate the spatial distribution of pesticide source strength $\hat{S}$ and economic effort $\hat{\theta}$ at the investigated groundwater location over three example years. We observe that regions with higher $\hat{S}$ also exhibit higher $\hat{\theta}$, indicating that the model allocates greater effort to areas with stronger pesticide sources. Over time, the average value of $\hat{S}$ decreases, representing the diminishing presence of pesticides in groundwater. Conversely, the computed local effort increases in a more marked way. The empirical application, based on real data, does not incorporate the optimal local effort recommended by the model. As a result, atrazine levels decrease based solely on the (absence of) localized treatment at the time. Consequently, the persistence of high pesticide levels in certain provinces, resulting in elevated $\hat{S}$ values, causes the outcomes of past groundwater treatment efforts to significantly deviate from the predictions of our model. The results suggest that, over time, policymakers' efforts to manage atrazine treatment, if any, failed to achieve a desired balanced spatial distribution across the country. Instead, it increased disparities in pesticide quantities nationwide.

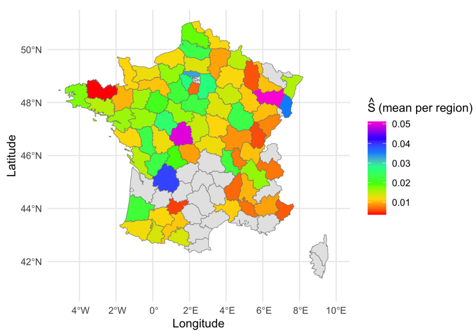
Consequently, the current effort is suboptimal, partly inefficient, and more expensive due to diminishing returns on effort.
In addition to analyzing the spatial variation in the model's computed effort to reduce pesticide presence — an aspect that directly influences social costs — it is equally important to examine the temporal dynamics of this effort, assessing how it evolves annually. In fact, the intensity with which it varies is extremely high. For example, in the Dordogne province in southwest France, the source term decreases from ≈ 0.06 in 2016 to ≈ 0.03 in 2022, while the effort value rises from ≈ 0.00005 in 2016 to ≈ 0.005. This indicates that the effort intensifies as pesticide levels decline, likely to meet stricter environmental targets. This behavior highlights the importance, stressed by the model, to act early in the application of the effort. Later application of the effort is going to reflect in higher effort needed to be able to meet the desired pesticide level for future generations. In the particular case of Dordogne, the computed effort to be applied starting seven years before the end of the simulation period and to meet the targeted pesticide levels is in fact around one hundred times lower than the one computed just one year before the final year. The model effectively captures how policymakers should adjust economic efforts to reduce pesticide exposure and ultimately achieve a predetermined level of residual pesticides in the environment. For each period, the intensity of effort corresponds to the differences in pesticide presence across geographical areas. However, the change in effort intensity from one year to the next varies based on the current pesticide levels and their distance from the target level that policymakers aim to leave for future generations. Failing to adhere to the recommended effort may result in a sharp increase in effort between years, leading to more costly and less effective treatments.



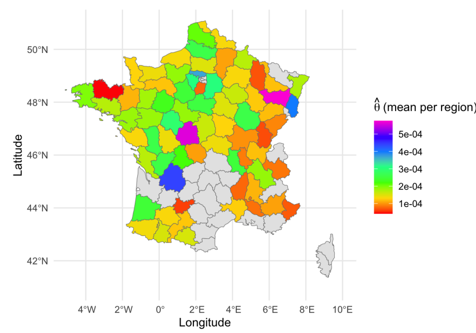
(a) Spatial values of $\hat{S}$ in 2016



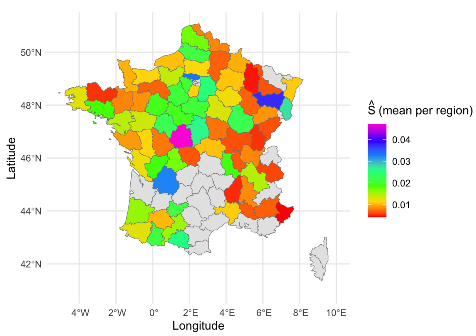
(b) Spatial values of $\hat{\theta}$ in 2016



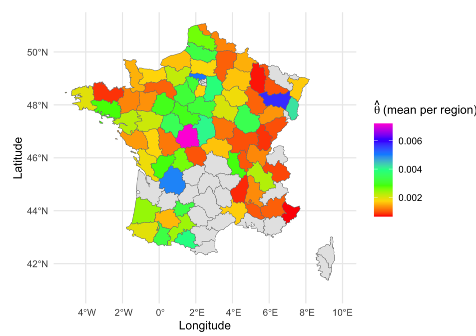
(c) Spatial values of $\hat{S}$ in 2019



(d) Spatial values of $\hat{\theta}$ in 2019



(e) Spatial values of $\hat{S}$ in 2022



(f) Spatial values of $\hat{\theta}$ in 2022

Figure 6: Spatial values of $\hat{S}$ and $\hat{\theta}$ in 2016, 2019 and 2022

7 Policy Implications and Conclusions

This study underscores the critical need for agricultural policies that are thoughtfully designed to balance health, environmental, and economic objectives. By integrating theoretical modeling, empirical analysis, and numerical estimation, we have adopted a comprehensive approach to address the challenges posed by pesticide persistence and its associated risks.

In this paper, we have introduced a novel space-time optimal control model that strategically balances the costs of transitioning from conventional to organic agriculture with the environmental and health benefits of reducing pesticide contamination. The dynamics of pesticide diffusion are captured through reaction-diffusion equations, a widely recognized mathematical framework for modeling the temporal and spatial spread of pollutants. This modeling approach provides significant insights into pollutant dispersion, population dynamics, and environmental interactions, offering a robust foundation for policy analysis.

The policymaker's objective function in our model is designed to address two pivotal dimensions. The first term represents a trade-off between the financial effort required to promote organic agriculture and the social costs associated with maintaining high pesticide levels. This term emphasizes the importance of weighing the immediate economic challenges of organic farming investments against the long-term societal benefits, such as improved public health and environmental quality. The second term focuses on the environmental outcome, specifically targeting the residual pesticide levels in the soil at the end of the planning horizon. This component ensures that the policy is not only economically viable but also environmentally impactful, reflecting the ultimate goal of achieving tangible reductions in pesticide contamination.

Another key contribution of this work lies in its empirical analysis, which uses French agricultural data to estimate the parameters governing the diffusion and decay dynamics of pesticides in groundwater. Atrazine, a pesticide known for its persistence and leaching properties, serves as a focal point for understanding the spatial and temporal impacts of pesticide contamination. The estimation of the diffusion (D_1) and decay (D_2) parameters, along with the computation of the source term (S) and control effort (θ), provides a deeper understanding of the mechanisms driving pesticide persistence and the decision process between conventional and organic agriculture investments.

From a policy perspective, our findings emphasize the importance of designing tailored, space-and-time-specific interventions that address the localized dynamics of pesticide diffusion and the varying costs of transitioning to organic practices. Optimal policies should prioritize areas where environmental and health risks are highest, while also considering the financial feasibility of organic investments. Additionally, our results suggest that a phased or regionally targeted approach to organic farming adoption may yield the most effective balance between economic and environmental outcomes.

Future research could further refine this framework by incorporating the effects of climate change on pesticide dynamics, as shifting weather patterns may alter diffusion rates and environmental interactions. Another promising avenue for exploration is the socio-economic impact of large-scale transitions to organic agriculture, particularly in terms of labor markets, food prices, and rural development. These extensions would provide a deeper understanding of the broader implications of sustainable farming practices, aiding policymakers in crafting strategies that promote both environmental resilience and public health while ensuring economic sustainability. In conclusion, the integration of optimal control theory with social and economic considerations offers a powerful tool for addressing the pressing challenge of pesticide contamination, paving the way for more sustainable agricultural systems.

Declaration of competing interest

There is no conflict of interest.

Data availability

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Appendix

The model estimates using the parameters obtained from the GWR with exponential kernel function are shown in Column 1 of Table A1. Instead, Column 2 shows the estimates obtained from the preferred model of Section 6.3 for direct comparison. When using the exponential kernel, the estimated decay coefficient D_2 and the time coefficient φ are statistically significant and similar in magnitude to those of the reference model. The only estimated coefficient that deviates notably is the diffusion coefficient D_1, although it is not statistically significant. Here, the R^2 is 0.4092, which is slightly lower than the 0.4097 of the considered model, indicating that it is less able to explain the variance in the difference in atrazine concentration levels.

	ΔP	ΔP
$\nabla^2 P$	-0.00313	0.00016***
	(0.00559)	(0.00002)
P	0.77254***	0.77018***
	(0.04081)	(0.04013)
t	-0.00102^{***}	-0.00101***
	(0.00008)	(0.00007)
Num. obs.	4,725	4,725
R^2	0.4092	0.4097
Adjusted R^2	0.3104	0.3109
Individual FE	Yes	Yes
Time FE	No	No
F Statistic	122.846***	184.828***
Note:	*p<0.1; **p<0.05; ***p<0.01	

Table A1: Diffusion model outputs using exponential kernel in the GWR estimation (left column) with respect to the considered model output (right column)

Figure A1 presents the values of R^2 for the estimated models using bandwidths ranging from 19 to 25 kilometers. Following the DGP approach, we selected the model with the highest R^2 value, which corresponds to a bandwidth of 20 and an R^2 value of 0.4097. Being the kernel fixed, the bandwidth represents the radius in kilometers from the considered groundwater location.

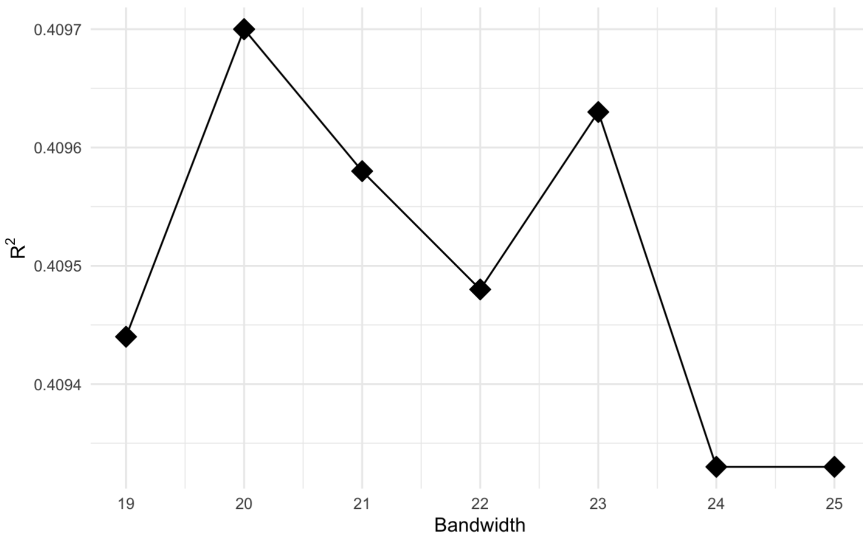

Figure A1: Model's R^2 for bandwidth selection

Figure A2 illustrates the distribution of the individual effects of each considered groundwater point. Most of them are concentrated around the value of 2.05, with some outliers above 2.10 and until almost 2.25. Figure A3 represents the values of the error terms with respect to the location and the year. Most of the error terms are concentrated around 0, with some higher level in the first years and lower levels towards the last one.

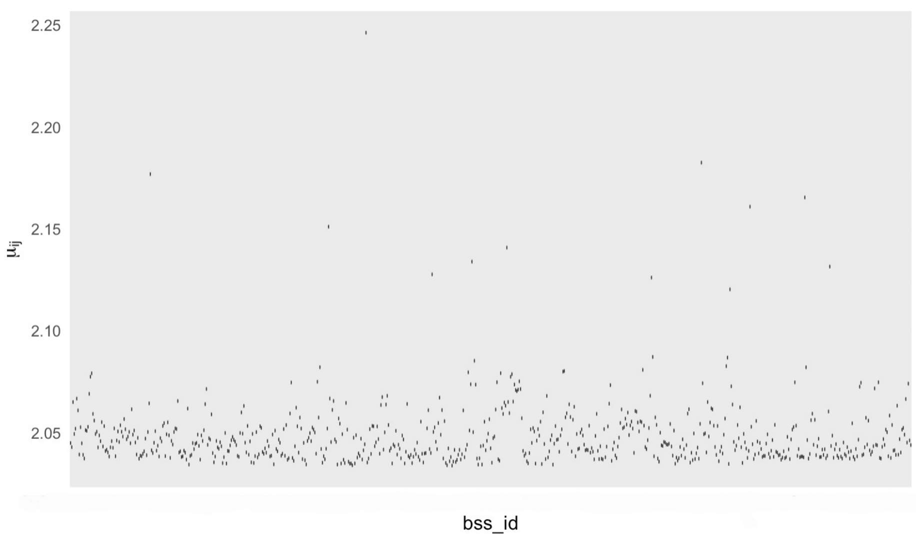

Figure A2: Distribution of the individual effects for each location

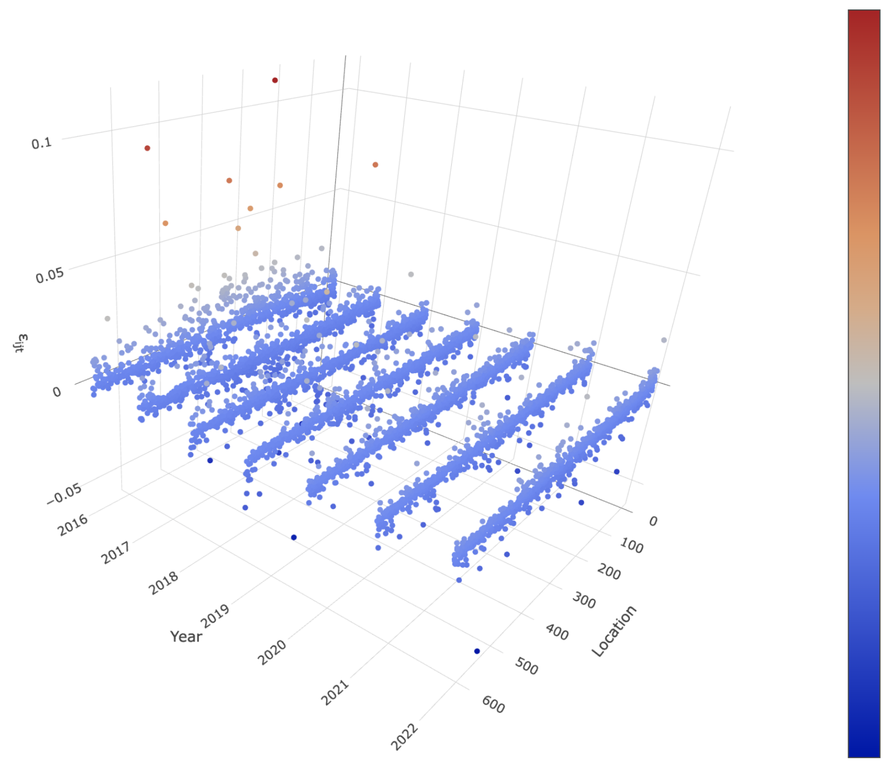

Figure A3: Error terms distribution for each location and year

Table A2 reports the descriptive statistics of $\hat{S}$ and $\hat{\theta}$, both globally and by year. Positive skewness values, observed both globally and across years, indicate that the distributions of the two variables exhibit long right tails. Moreover, the kurtosis values suggest that the distributions deviate from normality: the values tend to cluster around the mean, yet outliers are present.

$\hat{S}$

	Global	2016	2017	2018	2019	2020	2021	2022
Mean	0.01736	0.02314	0.01724	0.01686	0.01681	0.01695	0.01571	0.01484
SD	0.01945	0.02572	0.01852	0.01787	0.01854	0.01875	0.01700	0.01731
Min	-0.00292	-0.00110	-0.00129	-0.00277	0.00065	0.00151	0.00140	-0.00292
Max	0.32809	0.32810	0.21888	0.18545	0.22149	0.23839	0.18584	0.18547
Median	0.01230	0.01669	0.01258	0.01192	0.01175	0.01234	0.01106	0.00998
Skewness	5.08622	5.44036	4.67552	4.10019	4.79154	5.12905	4.51855	4.60249
Kurtosis	45.58912	47.99545	37.24287	28.08199	38.60647	44.32468	33.20821	33.28703

$\hat{\theta}$

	Global	2016	2017	2018	2019	2020	2021	2022
Mean	0.00058	0.00002	0.00003	0.00008	0.00019	0.00046	0.00101	0.00227
SD	0.00134	0.00002	0.00004	0.00008	0.00021	0.00050	0.00109	0.00265
Min	-0.00045	-0.00000	-0.00000	-0.00001	0.00001	0.00004	0.00009	-0.00045
Max	0.02837	0.00028	0.00044	0.00088	0.00249	0.00640	0.01191	0.02837
Median	0.00013	0.00002	0.00004	0.00006	0.00013	0.00033	0.00071	0.00153
Skewness	7.90535	5.44036	4.67552	4.10019	4.79154	5.12905	4.51855	4.60249
Kurtosis	106.30990	47.99545	37.24287	28.08199	38.60647	44.32468	33.20821	33.28703

Table A2: Descriptive statistics for $\hat{S}$ and $\hat{\theta}$

Figure A4 shows the density distribution of $\hat{S}$ and $\hat{\theta}$ using histograms and a density function. The graphs support and illustrate the findings from the descriptive statistics. The distributions of the estimated values are concentrated around their means. In particular, while the density of $\hat{S}$ becomes more concentrated over time—reflecting the standardization of the source term—the values of $\hat{\theta}$ become more dispersed and larger, indicating an increasing effort in organic agriculture over time. The presence of longer positive tails is also evident.

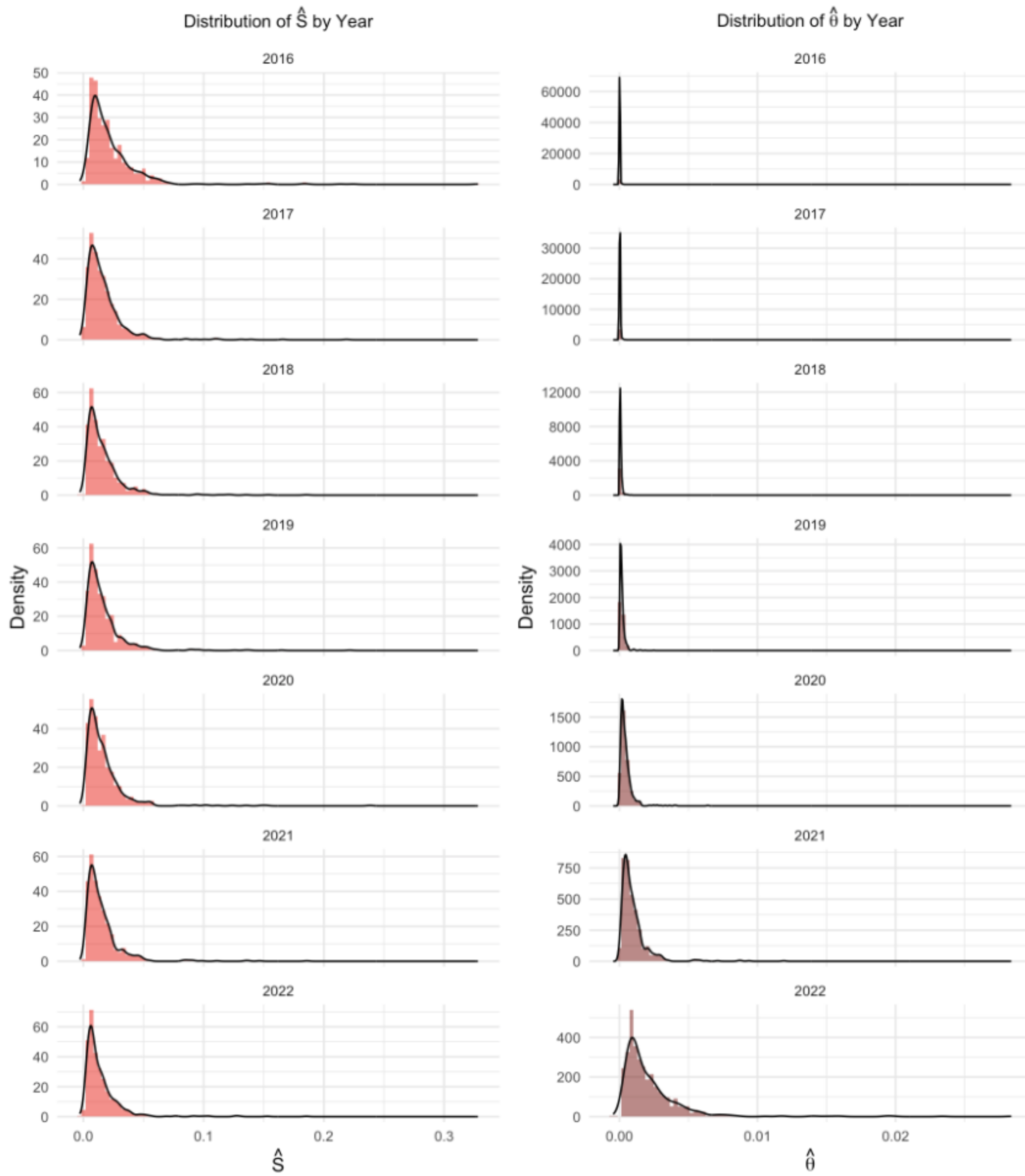

Figure A4: Distribution of $\hat{S}$ and $\hat{\theta}$

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