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To cite this article: Wissam Mansour Odah Al-Waeli *et al* 2024 *IOP Conf. Ser.: Earth Environ. Sci.* **1371** 032003

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Thiamethoxam Behaviour Modelling in the Clay Soil

Wissam Mansour Odah Al-Waeli [1], Alaa Hassan Al-Farttoosy[2] and Iman Mussa Omran[3]

[1-3]Department of Plant Protection, College of Agriculture, University of Basrah, Basrah, Iraq.

[1]E-mail: wissam.mansour@uobasrah.edu.iq
[2]E-mail: iman.omran@uobasrah.edu.iq
[3]E-mail: alaa.hassan@uobasrah.edu.iq

Abstract. Because all pesticides are poisons that are intentionally released into the environment, pesticide behaviour is significant. It is necessary to consider the chemical and physical properties of pesticides in order to comprehend the causes of poorly executed pest management. The results showed that the equilibrium constant of Thiamethoxam was achieved between 60 to 180 minutes. The kinetic reaction explained that Thiamethoxam is subjected to the second order with a rate constant of 0.0017 mg mimute^{-1}. Moreover it is more fitting to the Freundlich model compared to the Langmuir model. The bF was recorded 0.02 with the correlation coefficient 0.9999, indicating that Thiamethoxam mobiles on non-ideal surfaces. As long as it was subjected to the second reaction kinetic order, the half-life was 566.4 minutes (0.39 day). In terms of Thiamethoxam distribution in the soil, the distribution coefficient Kd was 0.22 mL g^{-1}, suggesting that Thiamethoxam tends to be less mobile in the soil.

Keywords. Thiamethoxam, Distribution Coefficient, First-order kinetic, Freundlich Isotherm, Langmuir Isotherm, Second-order kinetic.

1. Introduction

Thiamethoxam is 3(-2-chloro=1, 3-thiazol-5-ylmethyl)-5methyl-1, 3, 5-oxadiazinan-4-ylidene (nitro) amine (Fig. 1). Its action on the nicotinic acetylcholine receptor has an impact on the central nervous system synapses in insects. It acts by touch, the stomach, and systemic activity; it is quickly absorbed by the plant and moves acropetally through the xylem [1]. Additionally, thiamethoxam is frequently used to control armoured scale insects in addition to scald insects[2].

The recommendation use any pesticide requires knowledge about its dissipation/persistence behaviour and confirmation through adsorption studies and information about the degradation rate. This assists in evaluating and predicting the environmental pesticide behaviour[3]. Neonicotinoid insecticides are among the most widely used insecticides globally. Their popularity stems from their high toxicity to invertebrates, ease of application, versatility, and long-term stability, ensuring their distribution to all targeted crop parts. However, these characteristics also increase the potential for environmental pollution and exposure to non-target organisms[4]. Environmental contamination and accumulation occur in agriculturally viable soil, soil water, surface runoff in water bodies, and the uptake of insecticides by non-target plants through their roots or dust deposition on leaves. Persistence in soil, water bodies, and non-target plants varies but can be prolonged; for instance, the half-life of

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IOP Conf. Series: Earth and Environmental Science **1371** (2024) 032003 doi:10.1088/1755-1315/1371/3/032003

neonicotinoid compounds in soil can exceed 1000 days, potentially leading to accumulation with frequent use. Moreover, these compounds can persist in woody plants for periods exceeding a year[5]. Accumulation occur in agriculturally viable soil, soil water, surface runoff in water bodies, and the uptake of insecticides by non-target plants through their roots or dust deposition on leaves. And the half-life of neonicotinoid compounds in soil can exceed 1000 days, Moreover, these compounds can persist in woody plants for periods exceeding a year [6].

In a stability and leaching study of thiamethoxam in soil under laboratory conditions, stability tests conducted under two levels of inoculation and three moisture regimes indicated that thiamethoxam persisted for over 90 days in all treatments, The compound exhibited increased stability under dry conditions, while the opposite[7].

The absorption behaviour of thiamethoxam in three types of grapevine-cultivated soils in India, irrigated using drip irrigation, obtained Freundlich model constants for absorption rates[8].

The movement of insecticides in soil has a significant impact on pest control failure and environmental pollution, as evidenced by a comprehensive study investigating the behaviour of glyphosate in soil columns, indicating that glyphosate concentrations gradually decrease over time. The data also suggested better compliance of glyphosate with the Freundlich model compared to the Langmuir model, indicating multi-surface behaviour for this pesticide [9].

The soil sorption coefficient Kd and the soil organic carbon sorption coefficient KOC of pesticides are basic parameters used by environmental scientists and regulatory agencies worldwide in describing the environmental fate and behaviour of pesticides, and are thus directly related to both environmental mobility and persistence[10].

Distribution coefficient values indicated that some pesticides exhibited higher mobility in soil, while others showed lower mobility. In mathematical models, some pesticides showed better compliance with the Freundlich model, while others aligned with the Langmuir model[11].

The current study aims to characterise the Thiamethoxam residues kinetic in the clay soil under using different mathematic modelling.

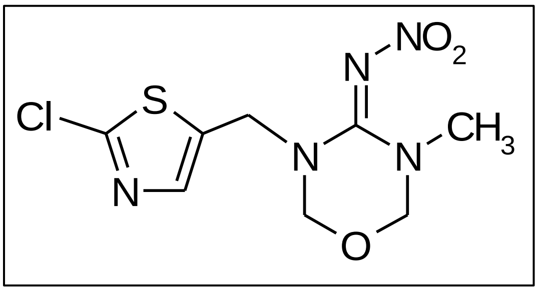

Figure 1. Chemical Structure of Thiamethoxam.

2. Materials and Methods

2.1. Chemicals

Thiamethoxam 25% WG is a Neonicotinoid insecticide that was purchased from the Al-Mugdadia Agricultural Company- Iraq- branch.

2.2. Batch Adsorption tests for Thiamethoxam

This experiment was done using 1000 g clay soil that was collected from the Date Palm orchard. This soil was air dried in the laboratory for three days. A 100 g placed into a 250 mL flask. These flasks were treated with 50 mL thiamethoxam solution containing 100 mg L^{-1}. These flasks were incubated in a shackled incubator at 150 rpm overnight. After that, the supernatant was withdrawn by 2 mL. Then those samples were centrifuged for 30 minutes at 3500 rpm. Lastly, a 0.22 filter was used to clean up the sample. Thiamethoxam concentrations were measured using the spectrophotometry at 250nm.

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2.3. Computes and Statistical Examination
Many kinetic modelling were applied to monitor Thiamethoxam residues in the clay soil, including: the kinetic reaction order, the coefficient of thiamethoxam distribution kd. Freundlich and Langmuir models were also used[12]. All calculations were performed using a Graph Prism 8.0.1 software- San Diego, California- USA.

3. Results and Discussion

3.1. Equilibrium Constant
In order to confirm that Thiamethoxam residues were in equilibrium after 24 hours, different Thiamethoxam supernatants were withdrawn from the flasks. The results in Fig (2) revealed that the neonicotinoid insecticide has been stable from 60-180 minutes. However it decreased after that to reach 40 and 39 mg L^{-1} after 4 and 5 hours respectively. The rate of Thiamethoxam decreasing scored 0.07 mg L^{-1} per hour. This indicates that Thiamethoxam is typically a slow movement from the soil to its solution. Biologically, this outcome demonstrated that Thiamethoxam can be absorbed into the soil and be released into solution after the soil's irrigation. This provides an eradication for the targeted pests due to the long activity of Thiamethoxam against the sucking insects. In this field[13], [14], reported that Thiophanate-Methyl and Carbendazim have been constant from 60 to 180 minutes.

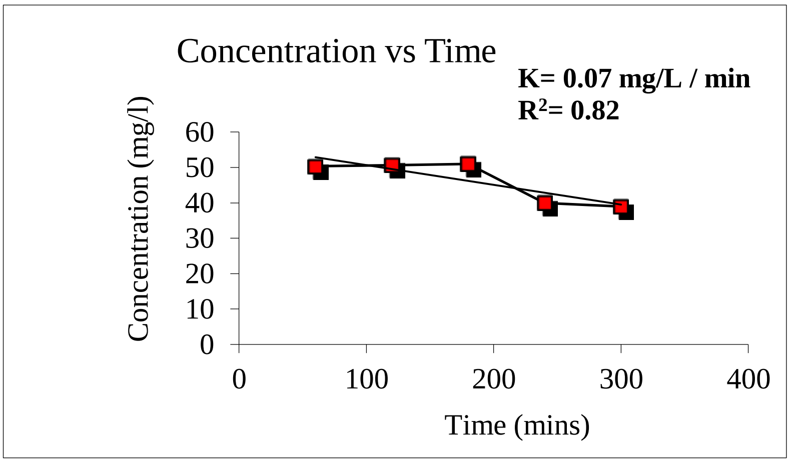

Figure 2. Equilibrium of Thiamethoxam residues in the clay Soil.

3.2. Thiamethoxam Kinetic Reaction
To compare which kind of Thiamethoxam kinetic reaction is subjected in the clay soil, the first and second order reactions have been evaluated. Fig. 3 compares the results obtained from the kinetic reaction analysis of Thiamethoxam. From the graph below we can see that Thiamethoxam is subjected to the second order reaction based on the R^2 values. It is also noted that the rate of Thiamethoxam dissipation was quite slow, with the rate scored 0.0012 and 0.0017 mg L^{-1} per hour. This point shows that the dissipation of Thiamethoxam dissipation in the soil depends on the concentration, which means when there is a double amount of Thiamethoxam residues, it requires a long time to be decreased compared to the first order reaction, which it does not rely on the concentration.
Similarly,[12] . found that Diazinon insecticide underwent the second order reaction. Moreover, in the previous study that was conducted by[15] pointed out the effect of insecticides in reducing the insects density underwent the second order reaction. On contrary, another studies were reported that some fungicide like Carbendazim, and Thiophanate-methyl were subjected to the Pseudo-first order[14] respectively; insecticides such as imidacloprid, indoxacarb, and lambda-cyhalothrin are subjected to the Pseudo-first order reaction, but Chlorantraniliprole underwent the Pseudo-second order reaction[11]. On the other hand, [9].illustrated that the herbicide glyphosate is subjected to the Pseudo-second order reaction.

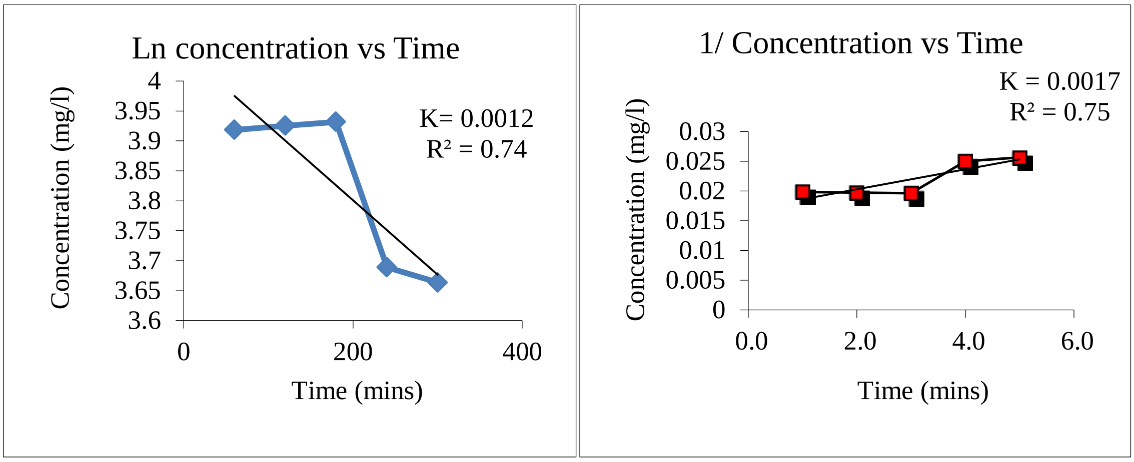

Figure 3. Thiamethoxam reaction of at A) First order B) Second Order.

3.3. Freundlich and Langmuir Models

Due to the role of Freundlich and Langmuir models in the knowledge of various chemical mobility in the soil, two mathematical equations that are employed[16]. Hence, from the data in Fig. 4A, apparent that Thiamethoxam insecticide is more fitting to the Freundlich model rather than the Langmuir model according to the R^2 value. The outcome of the Freundlich model for the Thiamethoxam is demonstrated by[17]. They demonstrated that a Freundlich isotherm is used to investigate non-ideal sorption on a heterogeneous surface since it's crucial to apply these models to comprehend the behaviour of thiamethoxam in soil.

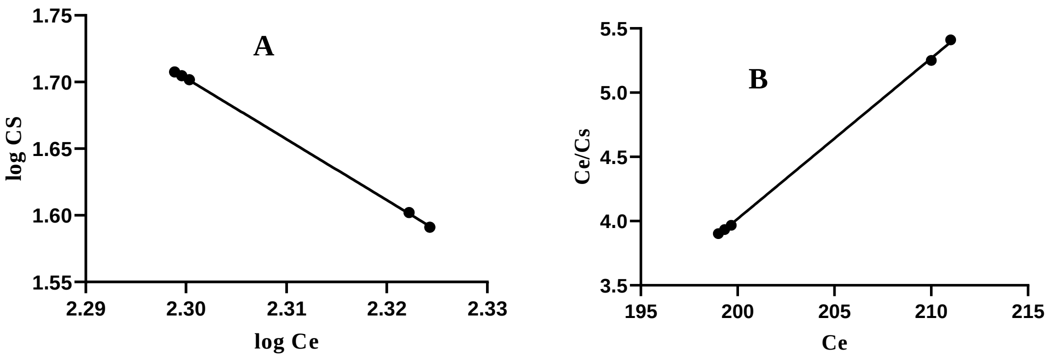

Figure 4. The sorption behaviour kinetic: A) Freundlich model, B) Langmuir model.

On the other hand, thiamethoxam appears to have been adsorbed on a single molecule if it conforms to the Langmuir model. Furthermore, the homogeneity of the surface-which is based on the lack of a sideways interaction-may have happened between neighbouring adsorbed molecules in particular when a single molecule occupies a single location on the surface[18].

Subsequently, the tables (1 and 2) are quite important and reveals the data of Thiamethoxam in the soil.

Table 1. Isotherm constant of Thiamethoxam adsorption based on the Freundlich model using linear regression.

Ln (Ce)	Ln (qe)	bF	Ln (aF)	R^2	Equation
2.67	12.21	0.02	0.066	0.9999	Y= -4.570X+12.2

Table 2. Isotherm constant of Thiamethoxam adsorption based on the Langmuir model using linear regression.

Ce	Ce/cs	KL	1/KL	R^2	Equation
167.9	21.00	0.1251	0.2701	0.9997	Y=0.1251x-21.0

According to the Thiamethoxam data assessment, some environmental parameters can be considered. It can be seen from the data in Table 3 that the time required to break down 50% of Thiamethoxam is different. It accounts for 802.5 minutes (0.55 day) and 566.4 minutes (0.39 day). The reason is that the availability of Thiamethoxam in the soil's solution although the rate of its degradation was quite slow. Whilst the half-life was quite fast in the case of Thiamethoxam is in the solution. In this field, Thiamethoxam can be dissipated relies on other factors like. For this reason, Thiamethoxam was subjected to the second reaction order. This order assumed that the chemical behaved under the second order.

Table 3. The Thiamethoxam rate constant and half-lives.

Parameter	Equilibrium constant	First-order	Second-order
half-lives (mins^{-1})	12.5	802.5	566.4
R^2	0.82	0.74	0.75

3.4. Coefficient of Distribution Kd

Further mathematical analysis of Thiamethoxam showed that Thiamethoxam has a Kd= 0.22 mL g^{-1}. This experiment detected that Thiamethoxam has little mobile and dispersive between the soil and its solution. Thus, it tends to be stable in soil or its solution. However there is a strong potential to uptake by plant roots due to it having a systematic function of insecticide. In addition to confirming this point, Thiamethoxam has a kind of persistence. Prior studies that have noted different Kd values. Many studies were conducted by [9], [13] confirmed diversity of pesticides in term of their coefficient distribution based on different factors. For example, they found that Thiophanate- methyl has scored Kd 6.5 mL g^{-1}, suggestion high-level mobile, whereas glyphosate has recorded Kd is 0.33 mL g^{-1}, which means less mobility. Lastly[11] additionally, there is a high degree of diffusion capability between the soil particles and the soil solution for indoxacarb and imidacloprid. The values for Kd are 5.25 and 1.30 mL g^{-1}, in that order. While lambda-cyhalothrin and chlorantraniliprole had scores of (0.639 and 0.562) ml g^{-1}, respectively, indicating that they are implicated in moderate soil mobility.

Conclusion

The present study was designed to monitor Thiamethoxam kinetic in the soil based on various mathematical modelling. The research has shown that thiamethoxam is constant during the first three hours. Furthermore, it underwent the second reaction order. This study also proved that Thiamethoxam fit to the Freundlich model rather than Langmuir. Accordingly, it takes a long time to dissipate its residues. This study proved that Thiamethoxam has less ability to distribute between soil and its solution.

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