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Original Article

Environmental partitioning of Vinclozolin and Zoxamide: An EQC level I investigation

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Abstract

Due to the large-scale use of fungicides in agriculture, it is important to understand how they partition into various environmental compartments. Understanding the partitioning of fungicides Vinclozolin and Zoxamide into multiple environmental segments is crucial in comprehending their effects on the environmental segments. One of the best methods for determining how chemicals enter the environment is through fugacity-based Equilibrium Criterion (EQC) model, which directly links fugacity with concentration and produces immediate findings. The Level I of this model assumes that the system is closed, the volumes of the compartments are fixed, the total amounts of chemicals distributed amongst the compartments are constant and the system is in an equilibrium steady state. While Zoxamide predominantly partitions in soil, Vinclozolin partitions nearly equally in soil and water, under Level I conditions. Aerosols have the greatest concentrations of Zoxamide and Vinclozolin followed by suspended sediment. Zoxamide is predicted to have a higher bioconcentration factor than Vinclozolin.

Keywords: Vinclozolin, Zoxamide, environmental modelling, EQC level I, fugacity

1. Introduction

The production of food is significantly impacted by pesticides. Pesticide might increase the number of times each year a crop can be raised on the specific piece of land while also protecting or boosting yields. This is critical in countries where food is scarce (Gomes *et al*., 2020). Pesticides protect crops from insects, fungi, weeds and other pests, depending on the dose and manner of exposure. Pesticides can be harmful to humans, with both short- and long-term health problems. Pesticide's toxicity varies according to its use and other aspects. The same chemical can have various effects depending on the dosage or the quantity of chemical to which a person is exposed. The exposure method such as ingestion, inhalation or direct skin contact can also affect the degree of toxicity. Populations which are at direct exposure to pesticide or fungicide are always at high risk. This covers everyone present during the delivery of pesticides and for a brief period later, as well as agricultural employees who apply pesticides (Damalas & Koutroubas, 2016).

Most people are exposed to far lower amounts of pesticide residues in their food and water because they do not live in an area where pesticides are utilised. Pesticides have various benefits and drawbacks. They diffuse through water, air, and soil. Pesticides also upset ecosystems. Pesticides often kill non-pest creatures. This can disrupt the environment. Different types of pesticides exist. We may divide them according to three broad qualifications. Organization of pesticides into categories is based on their chemical composition, the pests they are effective against, and the routes through which they enter the body (Blair, Ritz, & Wesseling, 2015; Constable, 1909; Eddleston *et al.,* 2002; Margni, Rossier & Crettaz, 2002; Nicolopoulou-Stamati, Maipas, Kotampasi, Stamatis, & Hens, 2016).

Aqueous solubility, vapour pressure, the air-water partition coefficient, molecular diffusivity, absorptivity and melting point are a few chemical characteristics of pesticides that affect their dispersion and transformation after they are released into the atmosphere (Su, Zhang, Cridge & Liang, 2019).

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Fungicides are primarily used to eradicate parasitic or entomopathogenic fungi as well as their spores. These are mainly listed as chemical based fungicides as well as natural based fungicides. This study has examined the distribution of both Zoxamide and Vinclozolin fungicides into various environmental-based compartments. EQC level I proposal based on fugacity has been taken for examining the spreading of both fungicides into each of the environmental sections. The environmental fate is examined by the results of EQC level I calculations. The key advantage of this strategy is that it produces immediate results that are easy to analyse and requires relatively little information (Mackay, 2004; Parnis &Mackay 2020). The main disadvantage is that it assumes a wide range of usual environmental conditions, which makes it less genuine and more similar to an experimental investigation in which reactions take place under controlled conditions. We have carried out such Level I studies on several pesticides (Thakur, Sharma & Qanungo, 2021).

Zoxamide is the chemical name for 3,5-dichloro-N-(1-chloro-3-methyl-2-oxopentan-3-yl)-4-methylbenzamild which is of benzamide class (EFSA Journal, 2016), Figure 1. Molecular formula of this fungicide is $C_{14}H_{16}Cl_3NO_2$. It is basically an oomycete fungicide that can be used for crops of mainly grapes and potatoes. It acts as an inhibitor of microtubule structure and inhibits cell division. It is mainly used to treat oomycetes fungus-like eukaryotic micro organisms, called oomycetes, as well as against some true fungi. Zoxamide is degraded biologically by anaerobic and aerobic conditions in the environment (Cai *et al*., 2015). It's mostly harmful to freshwater fishes (rainbow trout, bluegill sunfish) while it has low toxicity to mammals (Pan *et al*., 2020).

Vinclozolin is a member of the dicarboximide class named as n (3-(3,5-dichlorophenyl)-5-methyl-5-vinyl oxazolidine-2,4-dione), Figure 2. The molecular formula is $C_{12}H_9Cl_2NO_3$. It is a non-systemic fungicide used to control various rots and blights caused by fungal pathogens, widely used on fruits, vegetables and wines, and effective against fungal plagues. Vinclozolin is broken down in the environment, biologically in anaerobic or aerobic condition. It is poisonous to rats as it has been seen to have anti androgenic activity (Zhang *et al*., 2020).

Both of these pesticides are widely used in agriculture. The environmental partitioning of these fungicides is being investigated utilising a fugacity-based EQC Model Level I method, which may be effective in predicting the destiny of a chemical in various environmental compartments.

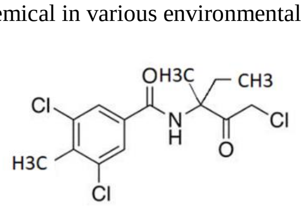

Figure 1. Structure of Zoxamide

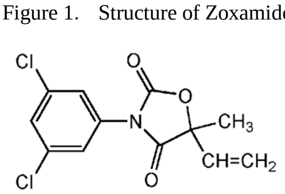

Figure 2. Structure of Vinclozolin

2. Methodology

The partitioning of these fungicides in the different compartments of the environment has been predicted using a fugacity-based EQC model Level I computation. These compartments include air, soil, fish, aerosols, sediments, water and suspended sediments. Level I models make various assumptions before performing computations (Cahill, Cousins & Mackay, 2003; Mackay & Paterson, 1981). These presumptions include that substances are inert, that they do not transfer across phases, the system follows steady state conditions and there is no chemical loss or degradation. The "escaping tendency" of a chemical species in a given phase is represented by the thermodynamic property known as fugacity (Guardo, Gouin, Macleod & Scheringer, 2018; Rong-Rong, Che-Sheng, Zhong-Peng & Xiao-Meng, 2012). EQC models use fugacity to determine the chemical fate in environmental compartments.

A number of studies illustrating the evaluation of chemical fate in the environment have been carried out using Level I, II, and III EQC models and reviewed (Mackay & Paterson, 1991; Mackay, Paterson, Cheung & Neely, 1985; Mackay, Paterson & Joy, 1983; Paterson, Mackay, Tam & Shiu, 1990; Wania & Mackay, 1999). The model originally proposed by Mackay (released in September 2004, Version 3.00, ©2004 Trent University) was used to carry out the Equilibrium Criterion Level I calculations with the EQC standard environmental parameters as shown below in Table 1 (Mackay, Guardo, Paterson & Cowan, 1996; Seth & Mackay, 2001).

In Mackay's model, there are four specified chemical classes depending on their vapour pressure and water solubility and Vinclozolin and Zoxamide belongs to the Type 1 chemical class. The physicochemical characteristics used to analyse the partitioning of these fungicides from the University of Hertfordshire's pesticide composition database are shown in Table 2.

The ability of a substance to dissolve in water is referred to as its water solubility. The pressure exerted by a liquid at its equilibrium surface is known as vapour pressure. It indicates the rate of evaporation. The process of volatilization of the chemical from water to air is indicated by Henry's law constant. It is determined by the ratio of solubility of the chemical to its partial pressure. The bioconcentration factor shows how a chemical accumulates in organisms. Subcooled vapour pressure represents the vapour pressure at which a substance is liquid when it is below its melting point and does not crystallise. The equation (1) describes the fugacity of chemical in a multicompartment system.

$$f = \frac{M}{\Sigma v_i z_i} \quad (1)$$

where *M* is number of moles of the chemical, in the i^{th} phase

$$c_i = f z_i \quad (2)$$

where C_i = concentration of chemical in i^{th} phase, *f*
= fugacity, *vi*
= volume of i^{th} phase, *zi*
= fugacity capacity of i^{th} phase

Table 1. EQC standard environmental parameters

Phase	Volume (m^3)	Density (kg/m3)	Organic carbon (g/g)	Fish lipid (g/g)
Air	1.00E+14	1.21	-	-
Aerosol	2000	2000	-	-
Water	2.00E+11	1000	-	-
Suspended particles	1.00E+06	1500	0.20	-
Fish	2.00E+05	1000	-	0.05
Soil	9.00E+09	2400	0.02	-
Sediment	1.00E+08	2400	0.04	-

Table 2. Physicochemical parameters of Zoxamide and Vinclozolin

Parameter	Zoxamide	Vinclozolin
Water solubility	0.68 g/m^3	3.40 g/m^3
Molar mass	336.64 $g.mol^{-1}$	286.11 g/mol
Vapour pressure Pa	1.3 x 10^{-5} Pa	1.60E-05 Pa
Melting point °C	159.5 °C	108 °C
Log K_{ow}	3.76	3.02
Data temperature	20°C	20 °C

$$Z_{air} = \frac{1}{RT} \quad (3)$$

$$Z_{aerosol} = z_a \times K_{qa} \quad (4)$$

where Z_{air} and $Z_{aerosol}$ are fugacity capacities of air and aerosol respectively

$$K_{qa} = \frac{6\times10^6}{P_L} \quad (5)$$

where K_{qa} is aerosol-air partition coefficient

$$P_L = Pexp\left[6.79\left(T_{\frac{M}{T}} - 1\right)\right] at\ T < T_M \quad (6)$$

P_L is subcooled vapour pressure.

$$z_w = \frac{S}{P} \quad (7)$$

where z_w is fugacity capacity of water, s is water solubility and p is vapour pressure.

Z_{soil} defined as

$$Z_{soil} = K_{soil} \times \rho_{soil} \times Z_w \quad (8)$$

ρ_{soil} = 2.4 kg/l

where ρ_{soil} is density of soil 2.4kg/l, k_{soil} is soil-water partition coefficient.

$$K_{soil} = K_{oc} \times foc(soil) \quad (9)$$

where K_{oc} is the organic carbon water partitioning coefficient, *foc*(*soil*)=fraction of organic carbon (0.02)

$$K_{oc} = 0 \cdot 41 \times K_{ow} \quad (10)$$

where k_{ow} is octanol water partition coefficient.

$$z_{susp.sed.} = K_{susp.sed.} \times \rho_{susp.sed.} \times z_w \quad (11)$$

where $\rho_{susp.sed}$ is the density of suspended sediment, 1.5 kg/l

$$K_{sus} = K_{oc} \times foc(susp) \quad (12)$$

where *foc*(*sus.sped*) is the density of suspended sediment, 1.5 kg/l

$$Z_{sed} = K_{sed} \times \rho_{sed} \times Z_w \quad (13)$$

where ρ_{sed} is the density of sediment, 2.4 kg/l

$$K_{sed} = K_{oc} \times foc_{(sed.)} \quad (14)$$

where $foc_{(sed.)}$ is fraction of organic carbon of sed, 0.4

$$Z_{fish} = K_{fish} \times \rho_{fish} \times Z_w \quad (15)$$

where ρ_{fish} is density of fish, 1.0 kg/l

$$K_{Fish} = 10^{log\ k_{ow}} \times L \quad (16)$$

where L is fraction lipid content of fish, 0.05

$$H = \frac{P}{S} \times M \quad (17)$$

where H is Henry law constant, p is vapour pressure, s is the water solubity.

All of these calculations were performed using EQC Level I software, which enables determining the quantity and concentration of these fungicides in different sections of the environment. The amount of these fungicides released in the environment was taken to be 100,000 kg (Matthies, Klasmeier, Beyer & Ehling, 2009).

3. Discussion and Results

With the use of equilibrium criterion (EQC) software, the computations involved the determination of fugacity capacity, and partition coefficient of individual environmental compartments. It also involved the calculation of concentration, percentage distribution and amount from which the distribution of Zoxamide and Vinclozolin fungicide into various compartments of the environment were determined. The air-water concentration ratio indicates how a chemical is susceptible from being removed from the atmosphere to water. As K_{aw} is very low, concentration of both the pesticides the air compartment should also be very low.

Table 3 contains the partition coefficients that were used in the subsequent calculations. Henry's law constants for these fungicides are very low, indicating that the chemicals have a tendency to remain in water and would have low concentrations in air (Mackay, Di Guardo, Paterson, Kicsi & Cowan, 1996). The high octanol water value of coefficient suggests that these fungicides are poorly soluble in water and that a high level of bioaccumulation is to be expected (Mackay

& Fraser, 2000). The high k_{oc} value suggests that these fungicides will be strongly adsorbed into the soil (Copaja, & Gatica-Jeria, 2021).

Table 3 shows that the partitioning of both the fungicides in air will be reduced because of the decreased vapour pressure. Calculations indicate that the air concentration of Zoxamide is minor (6.30E-13 mol.m^{-3}). In Table 4, the highest concentration is likely to be in aerosol section (1.15E-02 mol.m^{-3}) followed by suspended sediment and water, i.e. 1.69E-04 mol.m^{-3} and 6.88E-05 mol.m^{3} respectively for Zoxamide.

Diagrammatic representations and the outcomes of Level I scenario for Zoxamide and Vinclozolin are expressed in Figure 3 and Figure 4. For Zoxamide, the soil compartment clearly has the highest amount, while the fish compartment has the least amount of it.

Figure 4 depicts the output of Vinclozolin simulation. The water compartment clearly contains the highest amount, while the least amount of it is in fish.

Figure 5 displays the amount of Zoxamide that was distributed into the various environmental compartments. According to the graph, soil and water contain the highest

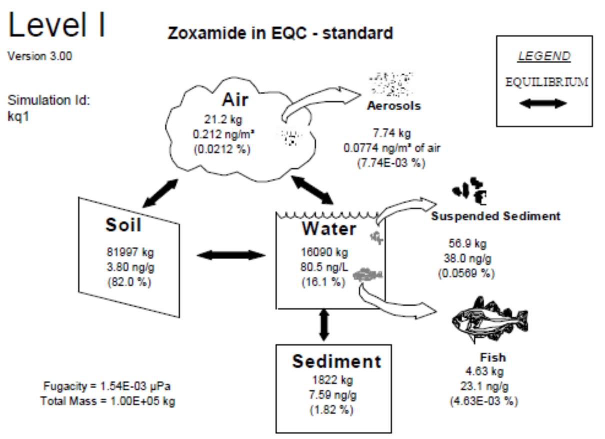

Figure 3. Schematic depiction of EQC Level-I modelling outcomes for Zoxamide

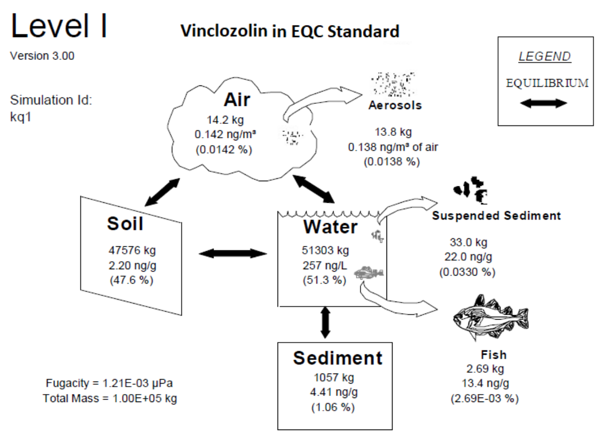

Figure 4. Schematic depiction of EQC Level-1 modelling outcomes for Vinclozolin

Table 3. Calculated Henry's law constants and partition coefficients of Zoxamide and Vinclozolin

Partition coefficients	Dimensionless Zoxamide	Dimensionless Vinclozolin	L/kg Zoxamide	L/kg Vinclozolin
Organic carbon-water	-	-	2359	429
Soil-water	113	20.60	47.20	8.59
Fish-water	288	52.40	288	52.40
Air-water	2.64×10^{-6}	5.52×10^{-7}	-	-
Sediment-water	226	41.20	94.40	17.20
Aerosol-air	1.82×10^{10}	4.88×10^{10}	-	-
Octanol-water	5754	1047	-	-
H	6.43x10^{-03} Pa.m³/mol	1.35x10^{-03} Pa.m³/mol		

Table 4. The spread of Zoxamide and Vinclozolin in the various environmental sections

Compartment	Fungicide name	Conc. (mol.m^{-3})	Amount (kg)	Percentage distribution
Air	Zoxamide	6.30E-13	21.2	2.12E-02
	Vinclozolin	4.95E-13	14.2	1.42E-02
Aerosols	Zoxamide	1.15E-02	7.74	7.74E-03
	Vinclozolin	2.42E-02	13.80	1.38E-02
Water	Zoxamide	2.39E-07	16090	16.10
	Vinclozolin	8.97E-07	51303	51.30
Suspended Silt	Zoxamide	1.69E-04	56.90	5.69E-02
	Vinclozolin	1.15E-04	33	3.30E-02
Fish	Zoxamide	6.88E-05	4.63	4.63E-03
	Vinclozolin	4.69E-05	2.69	2.69E-03
Soil	Zoxamide	2.71E-05	81997	82.0
	Vinclozolin	1.85E-05	47576	47.60
Sediment	Zoxamide	5.41E-05	1822	1.82
	Vinclozolin	3.70E-05	1057	1.06

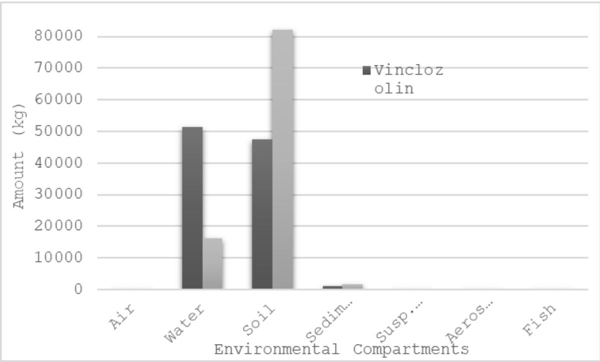

Figure 5. Amounts of Zoxamide and Vinclozolin in various environment compartments

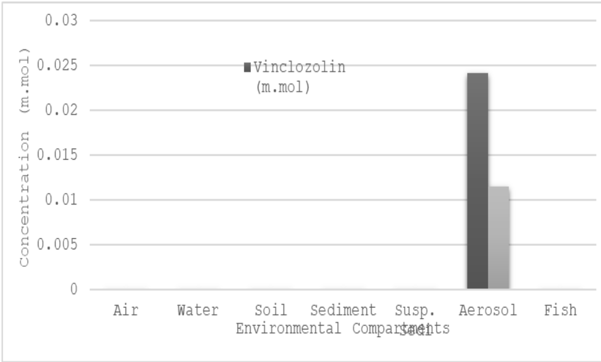

Figure 6. Concentrations of Zoxamide and Vinclozolin in various environmental compartments

amounts of Zoxamide. There is also a trace of Zoxamide in the sediment compartment. Remaining compartments contain negligible quantities of Zoxamide. Figure 5 also depicts the level of Vinclozolin in the various environmental sections. According to the graph, soil and water contain the highest amounts of Vinclozolin. Vinclozolin is also present in small amounts in the sediment compartment, and in negligible amounts in the other compartments.

The Zoxamide and Vinclozolin concentrations in different environmental compartments are presented graphically in Figure 6. The highest concentrations of both the pesticides are predicted to be in the aerosol compartment with minor concentrations in suspended sediment. Rest of the compartments contain insignificant concentrations. The bioconcentration factor, which is the ratio of concentration in fish to concentration in water is predicted to be 288 for Zoxamide, nearly six times that of Vinclozolin, 52. However, both the values are low and suggest that they are likely to concentrate in fish in small amounts.

In Figure 7, the pie chart depicts the relative distribution of Zoxamide pesticide in three compartments. According to the calculation the fraction of Zoxamide in soil is 82%, with 16% in water and 2% in sediment.

Figure 8 is a pie chart depiction of Vinclozolin distribution in the three main sections: water, soil, and sediments. The water and the soil compartments have nearly equal percentages of Vinclozolin at 51% and 48% respectively, and a minor amount (1%) is in sediment.

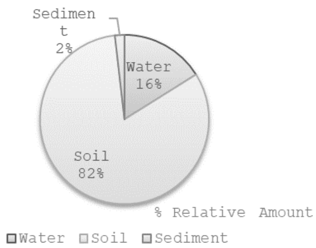

Figure 7. Relative distribution of Zoxamide in the different environmental compartments

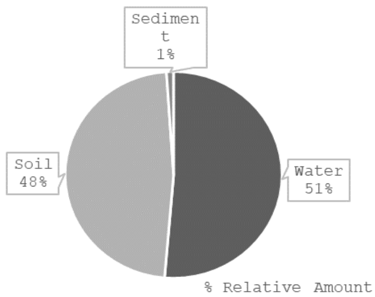

Figure 8. Relative distribution of Vinclozolin in the different environment compartments

4. Conclusions

Using the Level I EQC model, it is estimated that the majority of Zoxamide will accumulate in soil and a smaller quantity in water, while Vinclozolin partitions nearly equally in water and soil. Both of the pesticides exist in minor quantities in sediment. Aerosols are predicted to contain high concentrations of both the pesticides and suspended sediments containing very low concentrations. The bioconcentration factors of both the pesticides are low, therefore they are anticipated to concentrate in fishes in only small amounts.

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