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Bioconcentration factor of fungicides in soybean grains

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A B S T R A C T

Controlling phytopathogenic fungi in soybean crops (*Glycine max* L) is necessary and requires several types of fungicides, however, some of these pesticides can accumulate in soybeans. The bioconcentration factor (BCF) is a metric that indicates the degree of affinity of a substance for an organism. The BCF of the fungicides azoxystrobin, cyproconazole, epoxiconazole, and pyraclostrobin in soybeans from plants grown in pots, were estimated. Estimation was performed from concentrations of fungicides observed in the soil solution and in soybeans. Soybeans were exposed to fungicides by applications of the fungicides in the soil contained in pots. The average quantified concentrations in the grain samples were 6.21 µg/kg (azoxystrobin), 45.25 µg/kg (cyproconazole) and 10.47 µg/kg (epoxiconazole). The experimental value of BCF of fungicides varied between 0.044 L/kg (azoxystrobin) and 0.175 L/kg (epoxiconazole). With the estimated BCF values, the hypothetical concentrations of the fungicides in the soil solution that could translocate in the plant and exceed the maximum residue limits (MRLs) in soybean were then estimated. These concentrations were 11.36 µg/ml (azoxystrobin), 0.82 µg/ml (cyproconazole), and 0.28 µg/ml (epoxiconazole). BCF values and the acceptable daily intake (ADI) values of fungicides allows to estimate the risk of consuming a quantity of soybeans that provides a fungicide human intake greater than the ADI.

Keywords: Bioconcentration factor, Pesticide, Food security, Plant, Uptake.

Fator de bioconcentração de fungicidas em grãos de soja

R E S U M O

O controle de fungos fitopatogênicos na cultura da soja (*Glycine max* L) é necessário e requer diversos tipos de fungicidas, porém, alguns desses agrotóxicos podem se acumular na soja. O fator de bioconcentração (BCF) é uma métrica que indica o grau de afinidade de uma substância por um organismo. Estimamos o BCF dos fungicidas azoxistrobina, ciproconazol, epoxiconazol e piraclostrobina em soja proveniente de plantas cultivadas em vasos. A estimativa foi realizada a partir das concentrações de fungicidas observadas na solução do solo e na soja. A soja foi exposta aos fungicidas, através da aplicação dos fungicidas no solo contido em vasos. As concentrações médias quantificadas nas amostras de grãos foram 6,21 µg/kg (azoxistrobina), 45,25 µg/kg (ciproconazol) e 10,47 µg/kg (epoxiconazol). O valor experimental do BCF dos fungicidas variou entre 0,044 L/kg (azoxistrobina) e 0,175 L/kg (epoxiconazol). Com os valores de BCF estimados, foram calculadas as concentrações hipotéticas dos fungicidas na solução do solo que poderiam translocar-se na planta e ultrapassar os limites máximos de resíduos (LMR) na soja. Estas concentrações foram de 11,36 µg/ml (azoxistrobina), 0,82 µg/ml (ciproconazol) e 0,28 µg/ml (epoxiconazol). Valores de BCF e da ingestão diária aceitável (IDA) de fungicidas permitem estimar o risco de consumir uma quantidade de soja contendo o fungicida que proporcionaria um valor de IDA superior ao aceitável.

Palavras-Chaves: Fator de bioconcentração, Pesticida, Segurança alimentar, Planta, Absorção.

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Factor de bioconcentración de pesticidas en granos de soja

R E S U M E N
El control de hongos fitopatogénicos en el cultivo de soja (*Glycine max* L) es necesario y requiere diversos tipos de fungicidas, sin embargo, algunos agrotóxicos que pueden acumularse en la soja. El factor de bioconcentración (BCF) es una métrica que indica el grado de afinidad de una sustancia por un organismo. Fue estimado el BCF de los fungicidas azoxistrobina, ciproconazol, epoxiconazol y piraclostrobina en soja proveniente de plantas cultivadas en macetas. La estimación fue realizada a partir de las concentraciones de fungicidas observadas en la solución del suelo y en la soja. La soja fue expuesta a los fungicidas a través de su aplicación en el suelo contenido en macetas. El promedio de las concentraciones en las muestras de grano fueron 6,21 µg/kg (azoxistrobina), 45,25 µg/kg (ciproconazol) y 10,47 µg/kg (epoxiconazol). El valor experimental del BCF de los fungicidas varió entre 0,044 L/kg (azoxistrobina) y 0,175 L/kg (epoxiconazol). Con los valores de BCF estimados se calcularon las concentraciones hipotéticas de los fungicidas en la solución solo que podrían translocarse a la planta y superar los límites máximos de residuos (LMR) en la soja. Estas concentraciones fueron 11,36 µg/ml (azoxistrobina), 0,82 µg/ml (ciproconazol) y 0,28 µg/ml (epoxiconazol). Los valores de FBC y de la ingesta diaria admisible (IDA) de fungicidas permiten estimar el riesgo de consumir una cantidad de soja conteniendo el fungicida, el cual proporcionaría un valor de IDA superior al aceptable.

Palabras clave: Factor de bioconcentración, Pesticida, Seguridad alimentaria, Planta, Absorción.

1. Introduction

Several studies have shown that cultivated plants can absorb pesticides and polluting organic compounds. In this context, in order to avoid significant economic losses in agricultural crops, it is often necessary to protect cultivated plants from phytopathogenic fungi using fungicides. However, these chemical substances can accumulate in leaves, fruits, or grains, causing significant economic losses due to the compromised quality of agricultural products containing fungicide residues (Angioni et al., 2003; Angioni et al., 2011; Cabizza et al., 2012; Cabras and Angioni, 2000; Fantke et al., 2012; Hjorth et al., 2011; Itoiz et al., 2012; Navarro et al., 2011). The soybean (*Glycine max* L), also known as the soya or soja bean, is a plant with very great agricultural and industrial possibilities. As a foodstuff it has been of prime importance in China and Japan since ancient times; to a great extent it supplies the population of these countries with the nitrogenous food needed in the diet. Asian rust is a disease caused by the fungus *Phakopsora pachyrhizi* that affects soybean plants, if it is not controlled there could certainly be significant losses in grain production from soybean plantations. The economic damage caused by this disease is the significant decrease in productivity due to the early defoliation of plants that prevents the complete formation of soybean (Yorinori et al., 2004; Yorinori et al., 2005). Due to climatic conditions and the spread of the fungus by the wind, Asian rust can occur in all the world's soybean producing regions (Godoy et al., 2013). According to Moura (2017), ideally, Asian rust may be controlled applying fungicide formulations containing triazoles and strobilurins. The combination of these two types of fungicides is able to prevent Asian rust by protecting plants with strobilurin and curing plants infected with triazole.

Mathematical models might predict and prevent high toxic substance levels in field crops (fruits, tubers, vegetables, and grains) treated with pesticides or cultivated in polluted soils and indicate that organic substances must be systematically monitored through good crop management programs. Several mathematical models have been developed to simulate organic substance uptake by plants (Trapp and McFarlane, 1995, Trapp et al., 2003, Trapp, 2007, Paraíba, 2007, Paraíba and Kataguiri, 2008).

One way to avoid economic losses due to contamination of agricultural products by pesticides may be to estimate the risk of contamination using metrics that indicate the relative affinity of pesticides for agricultural products. The bioconcentration factor (BCF) of a substance in an organism is a numerical value that expresses the relative partition of the substance between the organism and the environment (Paraíba, 2007). Thus, BCF is a metric that indicates the degree of affinity of substances for organisms and can be used in the analysis of the risk of contamination of agricultural products by pesticides. In estimating the risk of contamination due to consumption of food obtained from soybeans plants grown with fungicides, bioconcentration factor (BCF) allows for the estimation of potential accumulation of fungicides in humans by daily consumption of soybeans in food. BCF and the acceptable daily intake (ADI) (mg/kg/body weight/day) of fungicides by daily consumption of soybeans (kg/day) allow us to estimate the risk of consuming a quantity of soybeans that contributes a daily intake value (DI, kg/day) of the fungicide greater than ADI. Thus, the prior knowledge of BCF of fungicides in soybeans may contribute to the proper agricultural management of these pesticides, preventing them from exceeding the maximum residue limit value (MRL, ml/mg) in soybeans.

Fungicide applications in soybean crops are always carried out by aerial spraying on the leaf surfaces of plants. The BCF estimate of fungicides in soybeans assumes that three successive applications of the fungicides are carried out and that the applied pesticides can reach the soil and contaminate the soil solution. Silva et al. (2019) quantified residues of various pesticides in soil solution samples from various agricultural areas in Europe. One study suggested that only a fraction (0.1%) of applied pesticides goes to targeted pests while the remainder spread to different compartments of the environment (Pimentel, 1995).

The modeling of the kinetic processes of absorption, elimination, and accumulation of pesticides by plants allows for the determination of BCF estimates of pesticides in stems, leaves, branches, fruits, grains, roots, and tubers (Trapp et al., 2003; Paraíba, 2007; Trapp, 2007; Trapp et al., 2007; Paraíba and Kataguiri, 2008). The main goal of this work was to estimate the BCF of the triazole fungicides cyproconazole, and epoxiconazole, as well as the strobilurin fungicides azoxystrobin and pyraclostrobin, in soybeans. The soybean plants were grown in a greenhouse using pots with soil. Soybeans were exposed to fungicides through three applications of the fungicides in the soil of pots with plants. Samples of soybeans and soil solution were used to determine levels of fungicide residues that were applied to the soil of pots. The analyzes of fungicide residues in soil solution samples were quantified by liquid chromatography with a diode array detector (LC-DAD) and the analysis of residues in soybean samples was carried out by gas chromatography coupled with mass spectrometry in series (GC-MS/MS).

2. Material and Methods

2.1. Hypotheses of fungicide bioconcentration in soybeans

The BCF was estimated on the basis that fungicides are dissipated in the soil-plant system according to first order kinetics, due to the growth of plants and the degradation of fungicides in the soil-plant system (Li, 2023; Li and Fantke, 2022; Wołejko et al., 2017; Xiao et al., 2021). It was assumed that the fungicides are non-ionic molecules (Queiroz et al., 2017) and that the processes of accumulation of the fungicides by the soybeans were through the transpiration flow of the soil solution by plants in the pots with fungicides in the soil solution (Krüger et al., 2013).

It was also assumed an absorption and elimination kinetics in steady state of the fungicide by the plant (Undeman et al., 2009) so that the BCF values were estimated by the quotient between the concentration of the fungicide in the soybean and the concentration of the fungicide in the soil (Melo et al., 2014).

2.2. Modeling of the bioconcentration factor (BCF) estimate of fungicides in soybeans

In a steady state absorption and elimination kinetics, the BCF is defined by the Equation 1:

$$BCF = C_{g(th)} / C_{w(th)} \text{ (L/kg)} \tag{1}$$

Where : $C_{g(th)}$ (µg/kg) is the concentration of the fungicide in the soybean at the time of soybean harvest and $C_{w(th)}$ (µg/L) is the concentration of the fungicide in the soil solution at soybean harvest time, where th (days) is the soybean harvest time.

Let t_0, t_1, and th (days) be the time intervals between the applications of the fungicides in the pots soil, where t_0 is the time interval between the first and the second application, t_1 is the time interval between the second and the third application, and th is the time interval between the third application and the harvest of soybeans. Let $C_{w(0)} = C_{w(0_1)}$ be the concentration of the fungicide in the soil solution after the first application. In the second application, the concentration of the fungicide in the soil solution will have been degraded until $C_{w(0_1)}e^{-kt_0}$ and will be increased by $C_{w(0_2)}$, the concentration of the second application, resulting in the Equation 2:

$$C_{w(1)} = C_{w(0_2)} + C_{w(0_1)}e^{-kt_0} \tag{2}$$

Where: k is the dissipation rate of the fungicide in the soil solution and was estimated using the expression k=0.693/t1/2, where t1/2 (day) is fungicide half-life in the soil solution.

In the third application, the concentration of the fungicide in the soil solution will have been degraded to $C_{w(1)}e^{-k(t_0+t_1)}$ and will be increased by the concentration of the third application, $C_{w(0_3)}$, the concentration of the third application, resulting in the Equation 3:

$$C_{w(2)} = C_{w(0_3)} + C_{w(1)}e^{-k(t_0+t_1)} \tag{3}$$

Consequently, the concentration of the fungicide in the soil solution of the pots on the day of the soybean harvest will be estimated by the Equation 4:

$$C_{w(th)} = C_{w(2)}e^{-k(t_0+t_1+th)} \tag{4}$$

The concentration of the fungicide in the soil solution for each application, $C_{w(0,1,th)}$ (µg/mL), was estimated by the Equation 5:

$$C_{w(0,1,th)} = \frac{10^{-3}m}{\mathrm{v}_{pot}(\rho_s K_D + \theta)} \tag{5}$$

Where:
v_{pot} (L) is the volume of the pot occupied by soil.
K_D (L/kg) is a constant representing the fungicide soil distribution coefficient estimated by $K_D = f_{oc}K_{oc}$, where f_{oc} (L/L) is the soil carbon organic volumetric fraction; K_{oc} (L/kg) is a constant representing the fungicide soil sorption organic carbon coefficient. ρ_s (kg/L) is the soil solution density. θ (L/L) is the soil water volumetric fraction in the soil field capacity. m (µg) is the mass of the fungicide applied in the soil given by $m = \mathrm{v}_{wp}C_{fcp}$, where v_{wfcp} (mL) is the volume of water used to dilute the formulated commercial product (mixture), and C_{fcp} (µg/mL) is the fungicide concentration in the formulated commercial product.

BCF of fungicides in the soybean was estimated by the use of a equation that calculates the BCF as a function of: the concentration of the fungicide in the soil solution at the time of harvest, the structural and physiological characteristics of the plant, and the physicochemical characteristics of the fungicides. Equations in Paraíba et al. (2010) were adapted to estimate BCF fungicides in soybeans.

The concentration of the fungicide in the soybeans can be estimated by the Equation 6:

$$C_{g(tc)} = \rho_g \frac{AQ_f C_{w(tc)}}{(B-k_s)}\left[e^{(-k_s t_c)} - e^{(-Bt_c)}\right] \tag{6}$$

Where:

ρ_g (L/kg) is the density of fresh soybean at harvest time.

Q_f (L/kg) is the total volume of water needed for the soy plants to produce 1.0 kg of fresh soybeans, estimated by $Q_f = 20d_w$, where d_w (L/L) is the soybean water volumetric fraction (Trapp et al., 2003).

A (constant of fungicide total uptake rate by soy plants) is defined by the Equation 7:

$$A = \frac{Q_f TSCF}{M_p} \tag{7}$$

Where: TSCF is the transpiration stream concentration factor of the fungicide given by $TSCF = 0.784e^{\left[-\frac{(\log K_{ow}-1.78)^2}{2.44}\right]}$, where $\log K_{ow}$ is the logarithm of the octanol-water partition coefficient of fungicide (Briggs et al., 1982; Brigs et al., 1983).

B (constant of fungicide total dissipation rate in soil solution) is defined by the Equation 8:

$$B = k_e + k_g + \frac{Q_x}{M_p(f_c k_{cw} + f_l k_{lw})} \tag{8}$$

Where: M_p (kg/pot) is the mature soybean plant total fresh biomass, Q_x (L/day) is the average daily soil solution volume transpired by soy plants per plots between the time of full flowering and the time of harvesting the fresh pods with soybeans. The plant dissipation rate was estimated by $k_e = 16k_s$ (1/day) (Juraske et al., 2008), k_g (1/day) is the growth rate of fresh pods with soybeans in the plant, f_c is the volumetric fraction of cellulose in the soy plants, f_l is the volumetric fraction of lignin in the soy plants, $k_{cw} = 10^{(\log k_{ow}-2.6)}$ (L/kg) is a constant representing the fungicide water-plant cellulose sorption coefficient, and $k_{lw} = 10^{(0.74\log k_{ow}-0.04)}$ (L/kg) is the fungicide water-plant lignin partition coefficient (Jonker, 2008).

2.2.1 Input data of BCF estimate of fungicides in soybeans

Three doses of the commercial mixtures of the fungicides azoxystrobin and cyproconazole, were applied. Residues of these fungicides in soil solution and in fresh pods with soybeans, were observed.

In order to estimate concentrations of fungicides in soil solution and in soybeans produced during the experiments, half-life times in soil solution for each of the fungicides was assumed. Half-life times used for the fungicides azoxystrobin, cyproconazole, epoxiconazole, and pyraclostrobin in soil solution were 56, 90, 90, and 37 days, respectively, (Tomlin, 2000).

Values of d_w, M_p, Q_x, f_c, f_l, and ρ_g were estimated at 0.67[a], 0.25 g/plant, 3.2 L/day, 0.46[b], 0.18[b], and 1.1 kg/L, respectively, ([a]http://tools.myfooddata.com/nutrition-facts/170174/wt1; [b]Rampoldi et al., 2011). Sorption coefficients values in the organic carbon of the soil, K_{oc}, of fungicides azoxystrobin, cyproconazole, epoxiconazole, and pyraclostrobin, which are used to estimate BCF in soybeans, were 589, 364, 1073, and 1100 (L/kg), respectively.

The logarithm of the octanol-water partition coefficient $(\log K_{ow})$ of fungicides azoxystrobin, cyproconazole, epoxiconazole, and pyraclostrobin are 2.5, 2.9, 3.44, and 3.99, respectively, (Tomlin, 2000). Doses of fungicides applied to the soil of the pots are shown in Table 1. The physical-chemical characteristics of soils used in the pots were: field capacity of $\theta = 0.30$ L/L, volumetric fraction of organic carbon $f_{oc} = 0.016$ kg/kg, and wet density $\rho_{sw} = 1.17$ kg/L.

2.2.2 Production and collection of soil solution and soybeans samples

The experiment was carried out in conditions required for planting, maintenance, development, and harvesting of soybeans from plants in pots. All soybean plants received three consecutive applications of the mixture of fungicides azoxystrobin and cyproconazole, and the mixture of the fungicides epoxiconazole and pyraclostrobin. Plants that received a mixture of azoxystrobin and cyproconazole did not receive a mixture of epoxiconazole and pyraclostrobin.

During the experiment, from sowing to harvesting of soybeans, the plants were kept in a greenhouse with dimensions of 6.40 m wide, 18.30 m long and 3.0 m high, and a total area of 117.12 m^2. The house was equipped with an automatic system to control light, temperature, and humidity, with an automatic drip irrigation system located in the pots, and with an automatic sprinkler irrigation system on the plants.

The soybean plants were grown in one hundred pots with a capacity of ten liters in which each pot, each containing seven kilograms of soil. Pots were kept in the greenhouse until the complete production of fresh pods with enough soybeans for sampling at harvest time. The soil used in the pots was extracted from an area with no history of pesticide use at the Experimental Station of Embrapa Environment (Jaguariúna, São Paulo, Brazil) located at latitude 22°41′S and longitude 47°W at a height of 570 m) and it is classified as Dystroferric Red Latosol, Oxisol (Latossolo Vermelho Distroférrico - LVdf; Santos et al., 2018)

Soy seeds of the Valiosa BRS-RR-C2 variety were grown in pots with soil. During the period between sowing the plants and harvesting the soybean pods with fresh soybeans, the following steps were performed: in the sowing, 10 soy seeds were planted per pot, the soybean seeds were all treated with rhizobium bacteria, when necessary, all soybean plants were kept in the greenhouse with artificial lighting from 3:00 am to 8:30 am in the morning and by 120 60-watt lamps, during sowing, sprinkler and drip irrigation were carried out, using a variable water layer, according to the development stages of the plants and according to local environmental changes, in order to maintain soil uniformity moisture, having as reference the field capacity, the irrigation depth varied between 5 and 10 mm daily, according to the water demand of the pots.

Germination and total seedling emergence occurred five days after sowing. For 51 days between germination and the beginning of flowering, we maintained irrigation and artificial lighting. Once a day, we maintained a 3 mm layer of water from the plant's development phase until the appearance of the first trefoil and applied three, or four, daily water drips to maintain soil moisture at field capacity. The time interval in which the irrigation system supplied water to the pots was 45 seconds. The water depth was defined using a soil moisture sensor. When the cotyledons of all plants were completely open, we thinned 6 plants and kept 4 plants per pot. The average weight of dry soil in pots without plants was 6.1 kg and the average weight of wet soil was 7.0 kg.

Three applications of fungicide mixtures were carried out, the first application in 45 days after planting in the soil pots, the second 15 days after the first application, and the third application 15 after the second application. The first application was carried out with the plants in the period of vegetative development, the second at the beginning of flowering, and the third at full flowering. Near the physiological maturation of the pods, 45 days after full flowering, we collected all the green pods with soybeans produced by the plants. The concentrations of the fungicides azoxystrobin, cyproconazole, epoxiconazole, and pyraclostrobin applied in the soil solution and the plant development stages are shown in Table 1.

Table 1 - Stages of development of soybean plants, dates of application of mixtures of azoxystrobin with cyproconazole and epoxiconazole with pyraclostrobin, and the doses applied to the soil of the pots with the soybean plants.

Stages	Vegetative	Beginning flowering	Full flowering
Days of application	**45 days after planting**	**15 days after the first application**	**15 days after the second application**
Fungicides	**(ug/mL)**	**(ug/mL)**	**(ug/mL)**
azoxystrobin	2.95	2.58	2.20
cyproconazole	1.12	1.12	1.10
epoxiconazole	1.09	0.90	0.83
pyraclostrobin	3.55	3.57	2.83

Concentrations observed in samples of applied doses were confirmed by analysis of residues in samples of syrup formulated with commercial products. Extractions of soil solution samples from the pots were performed using vacuum pumps applying a pressure of 75 kPa. The soil solution samples were collected by soil solution extractors with the aid of appropriate syringes and stored in a cold chamber for further analysis of fungicide residues. All samples were sent for analysis of residues at the Analytical Residues and Contaminants Center of Embrapa Environment.

Soil solution samples were collected eight hours before each application and eight hours after each application of the fungicides. The extraction of soil solution was interrupted when the volume of soil solution reached 100 ml in the extractor collector. Three extractors were installed in three pots with soil and plants: one extractor in a pot without applications of fungicides, one extractor in a pot with applications of the mixture of azoxystrobin and cyproconazole, and one extractor in a pot application of the mixture of epoxiconazole and pyraclostrobin. Collections of soil solution samples were carried out from the third application until the collection of fresh pods with soybeans. Regardless of the treatment, each pot with four soybean plants produced an average of 120 g of fresh pods with soybeans.

2.3. Determination of fungicide in the samples

2.3.1 *Reagents and chemicals*

Azoxystrobin standard was purchased from Chem Service Inc. (USA). Cyproconazole, epoxiconazole and pyraclostrobin standards were purchased from Fluka (Germany). All analytical standards were of > 99% purity. Ethyl acetate was purchased from Scharlau (Sentmenat, Spain), methanol and acetonitrile HPLC grade from Tedia (Fairfield, OH, USA). Glacial acetic acid (reagent grade) was purchased from J. T. Baker (Mexico). Ultrapure water was produced in the laboratory using a Milli-Q Advanced system from Millipore (Bedfore, MA, USA).

The salts used in QuEChERS extraction method were anhydrous sodium acetate acquired from Sigma-Aldrich (St. Louis, MO) and anhydrous magnesium sulfate $MgSO_4$ from Sigma-Aldrich (Japan). For the cleanup step, Bondesil-PSA 40 µm from Agilent (USA) and DSC-18 SPE from Sigma-Aldrich (Bellefonte, PA, USA) were used.

2.3.2. *Standard stock solutions*

Individual standard stock solutions at a concentration of 1000 µg/mL and intermediate solutions (10 µg/mL) were prepared in HPLC grade methanol. From these solutions, dilutions were prepared for the construction of analytical curves in ethyl acetate solvent for injection in the gas chromatograph or in acetonitrile/water (50:50 v/v) for injection in the liquid chromatograph.

2.3.3. *Determination of concentration of fungicides in the soil solution*

In order to quantify the active ingredients in soil solutions containing the commercial fungicides azoxystrobin and cyproconazole (Priori Xtra®, from Syngenta) or epoxiconazole and pyraclostrobin (Opera®, from Basf), aliquots of these solutions were collected and registered by the Analytical Residues and Contaminants Center of Embrapa Environmental. All samples were stored at -20ºC until the analysis. The samples were thawed and 15 mL were submitted to concentrations in Heidolph's rotary evaporator, with a bath temperature of 40ºC. After evaporating to dryness, the extract was resuspended in 1 ml of mobile phase acetonitrile/water (50:50, v/v) and filtered through a 0.45 µm membrane.

The analysis of fungicides in the samples were performed in Shimadzu Prominence 20A liquid chromatograph with SPD-M20A detector (Photodiode Array detector), using an Zorbax Polaris C-18 150x2.0 mm, 3 µm particle size, HPLC column from Agilent. A flow rate of 0.5 ml/min and the gradient elution mode were used. Detection was performed using a wavelength at 220 nm for azoxystrobin and cyproconazole and 210 nm for epoxiconazole and pyraclostrobin. Quantification method was performed by external standardization. Determination of limits of detection (LOD) and limits of quantification (LOQ) were performed at a signal-to-noise ratio of 3:1 and 10:1, respectively. Limits of detection, LOD (µg/kg), and limits of quantification, LOQ (µg/kg), of the analytical method are presented in Table 2.

2.3.4. *Determination of fungicide residues in soybean*

The preparation of the extract containing the fungicides was performed by the extraction with appropriate solvents, followed by a purification phase. The purified material was analyzed by gas-liquid chromatography through which the detection and quantification limits were established. Details of the procedures are described below.

Sample preparation: samples of soybean pods were received and registered at the Analytical Residues and Contaminants Center of Embrapa Environment and stored in a freezer at a temperature of -20ºC. The soybeans were removed from the pods manually, grinded in an industrial processor (model R3 Plus, Robot Coupe) and stored in a freezer at -20ºC until the analysis. The method used to extract the fungicides from the matrix was adapted with modifications from Gouvêa et al. (2015).

Two grams of grinded soybean samples were weighed in Falcon tubes (50 mL) and 3 mL of milli-Q water were added, waiting for 15 minutes. Then, 10 ml of acetonitrile containing 1% acetic acid were added and this solution was stirred for 1 minute using a vortex. After that, 6.0 g of magnesium sulfate and 1.5 g of sodium acetate were added with vigorous stirring for 1 minute. The extract was centrifuged at 4000 rpm for 10 minutes. For the cleanup step, 7 ml of the supernatant were collected and transferred to a Falcon tube containing 0.3 g of magnesium sulfate, 0.3 g of PSA and 0.3 g of C18 (Discovery – 18).

A new centrifugation was performed at 4000 rpm for 10 minutes. A volume of 3 ml of the supernatant was transferred to a concentrator tube. The extract was evaporated to dryness under nitrogen flow and redissolved with 500 µL of ethyl acetate, then injected in gas chromatograph coupled to a triple quadrupole mass spectrometer (GC-MS/MS).

Instrumental analysis: quantifications of residues were performed in a GC 7890A (Agilent), with a Gerstel KAS 4 PTV injector, a CTC Analytics auto-sampler coupled to a Waters Quattro Micro MS/MS (Micromass) detector. The column used was DB-5MS J&W Scientific 30 m X 0.25 mm X 0.25 µm, with He carrier flow of 1.0 mL/min. The oven temperature was 50ºC for 1.5 min, with a gradient of 15ºC/min up to 200ºC, remaining at that temperature for 2 minutes and 15ºC/min up to 300ºC, remaining the temperature for 8 minutes. The injection was performed in PTV (Programmed Temperature Vaporizing) in solvent vent mode, with an injection volume of 3 µL.

The injector programming was 50ºC of initial temperature, maintained for 0.30 min and after the valve was opened, the injector temperature was increased to 280ºC, at a rate of 12ºC/s for 27 minutes. In the mass spectrometer, the IE (electron ionization) source was operated with ionization energy of 70 eV with a temperature of 200ºC and the interface with a detector of 280ºC. The collision gas was argon 2.5x10^{-3} mBar. For each pesticide, two transitions were monitored. One for quantification and the other one for confirmation. The collision energy (EC) was adjusted to ensure greater sensitivity of analysis. Thus, the following transitions were monitored: azoxystrobin (344> 329 - EC 15V and 344> 328- EC 25V), cyproconazole (222> 125-EC 15V and 222> 82 –EC 5V), epoxiconazole (192> 138- EC 15V and 192> 111 - EC 15V) and pyraclostrobin (132> 77-EC 15 V and 164> 132-EC 10V).

Validation: validation of the analytical method for the determination of fungicide residues in soybeans followed the determinations of the protocol SANTE/11813/2017, as described below.

*Selectivity: s*electivity was performed by visual comparison of the chromatograms of the reagents blank, the standard in solvent, the control sample (matrix free of fungicides). No interference was observed in the fungicide retention times.

Linearity: Curves in the solvent and in the matrix were obtained using at least 5 (five) concentration points in triplicate. The determination coefficient (r^2) was equal to or greater than 0.99. The matrix effect for each analyte was analyzed. A matrix effect was observed with increased signal for epoxiconazole and cyproconazole and signal suppression for pyraclostrobin. For azoxystrobin, no significant effect was observed. Thus, to circumvent this problem, we worked with a curve in the matrix during validation and analysis.

Detection and quantification limits: the limit of detection (LOD) of the method was calculated as the lowest concentration with a signal/noise ratio of 3. The limit of quantification (LOQ) was established as the lowest concentration that was validated with acceptable accuracy and precision for each pesticide. LOD values were 1.00 µg/kg for azoxystrobin, cyproconazole and epoxiconazole, and 2.0 µg/kg for pyraclostrobin. LOQ values were 5.0 for all fungicides. Limits of detection, LOD (µg/kg), and limits of quantification, LOQ (µg/kg) of the analytical method used for residual fungicides determination in soybean samples are presented in Table 3.

3. Results and Discussion

The estimated concentration values and the determined concentration values (in soil solution and in soybeans) have numerical adhesions and are the same in orders of magnitudes. Evidently, in terms of limits of detection and quantification, the observed concentrations depend on the analytical capacity of the chromatographic method adopted in the analysis of residues in soil solution and in the soybeans.

The estimated concentrations of fungicides in soil solution and concentrations observed by analysis of residues in soil solution samples are shown in Table 2. The results were demonstrated with basis to soybeans exposition to the pesticides through three applications in the soil of pots with plants and with basis on the harvest period. It was observed that azoxystrobin was the fungicide that presented the highest concentration in the soil solution during the harvest period, as well as presenting the lowest LOD and LOQ values.

Table 3 presents estimated concentrations of fungicides in soybeans, the estimated BCF value of fungicides in soybeans, the concentrations observed by analysis of residues in soybeans and the observed value of BCF of the fungicides in soybeans.

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Table 2 - Fungicide concentrations of mixtures of azoxystrobin with cyproconazole and epoxiconazole with pyraclostrobin estimated in the soil solution by model and observed by analysis of residues in soil solution samples from the pots with soybean plants.

Table 1 experiment	$C_{w(0)}$ Dose one Estimated	$C_{w(0)}$ Dose one Observed	$C_{w(1)}$ Dose two Estimated	$C_{w(1)}$ Dose two Observed	$C_{w(2)}$ Dose three Estimated	$C_{w(2)}$ Dose three Observed	$C_{(th)}$ Harvest Estimated	$C_{(th)}$ Harvest Observed	LOD	LOQ
Fungicides	**(ug/ml)**	**(ug/ml)**	**(ug/ml)**	**(ug/ml)**	**(ug/ml)**	**(ug/ml)**	**(ug/ml)**	**(ug/ml)**	**(ug/ml)**	**(ug/ml)**
azoxystrobin	0.17	0.35	0.32	0.25	0.45	0.78	0.37	0.14	0.0001	0.0002
cyproconazole	0.07	0.10	0.23	0.18	0.34	0.27	0.30	0.07	0.0008	0.0020
epoxiconazole	0.20	0.14	0.30	0.02	0.35	0.01	0.31	0.06	0.0006	0.0018
pyraclostrobin	0.04	< LOD	0.06	< LOD	0.06	< LOD	0.04	< LOD	0.0008	0.0080

Table 3 - Fungicide concentrations of azoxystrobin with cyproconazole and epoxiconazole with pyraclostrobin in soybean grains estimated and observed by analysis of residues in soybean grain samples. BCF estimated of fungicides in soybean grain and BCF determined in by quotient between the concentration of the fungicides observed in the soil solution and concentrations of the fungicide observed in soybean grains.

	$C_{soybean\text{-}grain}$ Estimated	$C_{soybean\text{-}grain}$ Observed	$BCF_{soybean\text{-}grain}$ Estimated	$BCF_{soybean\text{-}grain}$ Observed	LOD	LOQ
Fungicides	**(ug/kg)**	**(ug/kg)**	**(L/kg)**	**(L/kg)**	**(ug/kg)**	**(ug/kg)**
azoxystrobin	21.03	6.21 ± 0.79 n = 2	0.06	0.044	1.00	5.00
cyproconazole	30.12	45.25 ± 35.09 n = 20	0.10	0.061	1.00	10.00
epoxiconazole	33.08	10.47 ± 6.5 n = 20	0.11	0.175	1.00	5.00
pyraclostrobin	1.10	< LOD	0.02	< LOD	2.00	100.00

Cyproconazole was the compound that demonstrated the highest accumulation in soybean-grains compared to the others fungicides, however its BCF was of a similar order of magnitude to that of azoxystrobin, and approximately only 35% of the BCF value of epoxiconazole. The latter was the fungicide that demonstrated the highest BCF value (0.175) and, together with azoxystrobin, demonstrated the lowest LOQ value (5 µg/kg).

In previous work we used a mathematical model that satisfactorily estimated the BCF and concentration of polycyclic aromatic hydrocarbons (PAH) in corn grains. The model was experimentally tested and validated, indicating which PAHs might accumulate in grains of corn plants cultivated in PAH-contaminated or SS-treated soils with sewage sludge for long periods (Paraiba et al., 2010). Other authors developed mathematical models in order to simulate organic substance uptake by plants

Fantke et al. (2011) modeled the dynamics of pesticide absorption by wheat plants and observed experimentally the absorption of the fungicides prochloraz, tebuconazole, chlorothalonil and cyproconazole and the insecticides deltamethrin and pirimicarb by wheat grains, Fantke et al. (2013) modeled the dynamics of pesticide absorption by plants and observed experimentally the absorption of dicamba (herbicide), carbaryl (insecticide), and cyromazine (insecticide) by leaves, stems and grains of wheat. Trapp and Eggen (2013) simulated the absorption of organophosphate pesticides and persistent organic pollutants by barley and carrot plants. Fantke et al. (2011) concluded that after foliar application, the human intake of these substances by the consumption of the contaminated grains would be of four orders of magnitude greater than the intake of residues of the same pesticides through the air.

Juraske et al. (2012) experimentally modeled and observed the accumulation of four fungicides (azoxystrobin, difenconazole, mancozeb and tebuconazole) and four insecticides (deltamethrin, imidacloprid, thiacloprid and thiamethoxam) by passion fruit plants and fruits. The authors concluded that the average values of pesticide residues observed in passion fruit at harvest time were below the maximum residue limits (MRLs) accepted in food by the European Union.

Xiao et al. (2021) estimated BCF values for about 700 pesticides and proposed parameterizations for including the effects of the periderm into a full plant uptake modeling framework. The authors compared the model estimates with measured data, showing that predictions agree with field observations for current use pesticides and some legacy pesticides frequently found in potatoes. In the present work, the agreement of predicted values with experimental values are compatible with Xiao et al. (2021) findings, and can be used for monitoring and legislation purposes. This would include the use of pesticides in the cultivation of grains important for the Brazilian economy such as corn, soybeans, rice, wheat and beans, among others.

Other practical application of the knowledge of the BCF value is that it is useful for calculating the hypothetical concentrations of fungicides in the soil solution (CHFSS), which are necessary to reach the maximum residue limits (MRLs) in soybeans. Table 4 presents an estimate of these concentrations.

Table 4 - Hypothetical concentrations of fungicide concentrations of mixtures of azoxystrobin with cyproconazole and epoxiconazole with pyraclostrobin in the soil solution (CHFSS) necessary to reach the maximum residue limits (MRL) in soybeans.

	azoxystrobin	**cyproconazole**	**epoxiconazole**
LMR (ug/kg)	500	50	50
CHFSS (ug/mL)	11.36	0.82	0.28

According to Hirakuri and Lazzarotto et al (2014), the per capita consumption of Brazilian soybeans is 17 kg/year (≈0.05 kg/day). In this study, samples of soybeans showed at most a concentration level of the cyproconazole fungicide of 45.25 µg/kg (Table 3). Considering the value of 45.25 µg/kg and a daily grain intake by an adult of 0.05 kg/day, it is possible to estimate the daily intake of cyproconazole DI (µg/day/kg) by the expression $DI = 0.05 \times C_g^{cyproconazole} / 70$, resulting in a daily intake of cyproconazole 0.032 µg/day/kg.

The acceptable daily intake (IDA) defined by the EPA (U.S. Environmental Protection Agency) of cyproconazole is 0.01 mg/day/kg. Consequently, a level of cyproconazole in soybeans of 45.25 µg/kg does not significantly compromise the quality of soybeans for human consumption. Thus, an individual of 70 kg of body weight who consumes 0.05 kg of soy per day (50.0 g) with this level of fungicide in the grain would be ingesting 0.002 mg of cyproconazole per day. This intake is much lower than the calculated IDA for this individual, since they could ingest up to 0.7 mg/day.

Assuming a 70 kg individual and the IDA (for 70 kg) of fungicides azoxystrobin, cyproconazole, and epoxiconazole of 1400, 700, and 210 ug/day, respectively, allows for estimating the maximum amount of soybeans (kg) that the individual should ingest so as not to exceed these values. Therefore, these maximum daily intake amounts for the three compounds were 225.44, 15.47, and 20.05 kg, respectively, according to the average concentrations quantified in soybeans. These were 6.21±0.79 ug/kg (azoxystrobin), 45.25±35.09 ug/kg (cyproconazole), and 10.47 ug/kg (epoxiconazole). Therefore, it is observed that the calculated values of maximum amounts of intake are far below the reality of consumption by the Brazilian population.

Similar to the present work, several authors have reported on the estimation of maximum daily intake amounts of xenobiotics in humans based on ADI values, BCF calculation and estimated concentration values in tissues of biological systems (Shiroma et al. 2021; Jonsson et al., 2019; Nunes et al., 2018). This gives the proposed mathematical model the possibility of use in assessing the risk of consumption of contaminants present in food, aiming to preserve the human health.

4. Conclusion

We estimated the values of bioconcentration factors (BCF) of fungicides azoxystrobin, cyproconazole, epoxiconazole, and pyraclostrobin in soybeans. Due to low persistence in the soil (half-life of 37 days) and high soil sorption (Koc = 1100) of fungicide pyraclostrobin in soil, we did not observe concentrations of pyraclostrobin in soil solution or in soybeans. The comparison between the BCF values, estimated and observed experimentally, showed that the method chosen to estimate the BCF value of fungicides in soybeans works satisfactorily and that it can be used to estimate the BCF of non-ionic fungicides in soybean.

The model was tested experimentally and validated, indicating which fungicides might accumulate in soybean of plants cultivated in soil containing the fungicides concentrations. The results obtained in the present work evidenced that fungicides applied in soils are able to attain the soybean and bioconcentrates in it. This fact might raise potential contamination risks to the food chain. However, in this work, a low risk for human health associated with the usual amount of soybeans ingestion was estimated. Therefore, additional research on this subject is of high concern and priority in order to achieve an ecologically correct and sustainable agriculture. More research is needed to know better the fungicides concentration ranges in soils and the consequent ecosystem impacts before using them as fungicides in agriculture.

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