Pesticide bioconcentration modelling for fruit trees

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Abstract

The model presented allows simulating the pesticide concentration in fruit trees and estimating the pesticide bioconcentration factor in fruits of woody species. The model allows estimating the pesticide uptake by plants through the water transpiration stream and also the time in which maximum pesticide concentration occur in the fruits. The equation proposed presents the relationships between bioconcentration factor (BCF) and the following variables: plant water transpiration volume (*Q*), pesticide transpiration stream concentration factor (TSCF), pesticide stem-water partition coefficient ($K_{Wood,w}$), stem dry biomass (*M*) and pesticide dissipation rate in the soil-plant system (k_{EGS}). The modeling started and was developed from a previous model "Fruit Tree Model" (FTM), reported by Trapp and collaborators in 2003, to which was added the hypothesis that the pesticide degradation in the soil follows a first order kinetic equation. The model fitness was evaluated through the sensitivity analysis of the pesticide BCF values in fruits with respect to the model entry data variability.

Key words: *Mangifera indica*; Paclobutrazol; Woody tree; Mathematical model; Fruits; Pesticides

Introduction

In general, the fruit tree production management includes the use of pesticides. Brazil is one of the world's greatest consumers and exporters of fresh fruits and fruit juices and ranks among the world's ten greatest pesticide users (Armas et al., 2005). Therefore, the Brazilian government concern about fruit quality related to pesticide concentration in fruits produced in Brazil and exported to other countries comes with the great expectations of Brazilian people and foreigners, consumers of fresh fruits.

Mathematical models might contribute to prevent concentrations of toxic substances in fruits of plants cultivated with pesticides and suggest that such substances must be systematically monitored in good agriculture practice programs. Several mathematical models have been developed to simulate the uptake of substances by plants (Fujisawa et al., 2002; Hung and Mackay, 1997; Matthies and Behrendt, 1995; Paterson and Mackay, 1995; Riederer, 1995; Trapp, 1995; Trapp and Matthies, 1995; Trapp and Matthies, 1998; Trapp and McFarlane, 1995; Trapp et al., 2003; Trapp and Pussemier, 1991). There are

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models developed to simulate leaf uptake (Trapp and Matthies, 1995), the ones to simulate root uptake (Trapp et al., 2003) and others to simulate both leaf and root uptake (Fujisawa et al., 2002).

A substance bioconcentration is defined as the concentration increase inside and/or on the surface of an organism (or in specific tissues) in relation to the substance concentration in the external medium (OECD, 1981). This research work aimed at modeling the bioconcentration and estimating the pesticide BCF value in fruits woody trees. The pesticides considered in this study are non-ionic organic compounds-degrading in the soil.

Material and Methods

Hypothesis for the FTM-p model

The pesticide bioconcentration modeling in fruits was developed from the original model named Fruit Tree Model (FTM), according to Trapp et al. (2003), and consisted of adding to it the hypothesis that pesticides degrade in the soil according to a first order kinetic equation. The FTM-p modeling supposes that the pesticide dilution processes due to plant growth, pesticide metabolism in the plant and pesticide degradation in the soil are described by first order kinetic equations. In both FTM and FTM-p models, the air/pesticide exchange by diffusion through the xylem/phloem, wood-bark and fruits were neglected. Thus, the pesticide transport into the plant was considered a passive process occurring through the plant transpiration stream. Both models were also supposed for woody and perennial fruit trees.

The FTM-p modeling from FTM model

Pesticide is transported via transpiration stream to all plant parts (roots, stems, leaves and fruits). In the plant, the pesticide is transformed through metabolic processes, diluted in function of plant growth a adsorbed in the woody parts. Thus, the pesticide total balance mass in the plant was calculated by (Trapp et al., 2003):

$$\frac{dm_{St}}{dt} \blacksquare Q \blacksquare C_{Xy} \blacksquare k_t \blacksquare k_G) \blacksquare M \blacksquare C_{St} \blacksquare \frac{Q \blacksquare C_{St}}{K_{StW}} \qquad (1)$$

where $m_{St} \blacksquare m_{St}(t)$ (mg day^{-1} ha^{-1}) is the pesticide total mass in the stem per hectare, Q (l day^{-1} ha^{-1}) is the water transpiration rate (transpiration stream) by plants, C_{Xy} (mg l^{-1}) is the pesticide concentration in the transpiration stream, M (kg ha^{-1}) is the stem total dry mass, k_t (day^{-1}) is the pesticide transformation rate in the stem, k_G (day^{-1}) is the plant growth rate, C_{St} (mg kg^{-1}) is the pesticide concentration in the stem and K_{StW} (l kg^{-1}) is the stem-water pesticide partition coefficient.

The pesticide concentration in the transpiration stream was estimated from the pesticide concentration in the soil solution and from the pesticide transpiration stream concentration factor, using the expression C_{II} [redacted] $TSCF$ [redacted] C_{I}, where C_{I} (mg l^{-1}) is the pesticide concentration in the soil solution and TSCF is the pesticide concentration factor in the transpiration stream. The TSCF value was estimated from the octanol-water partition coefficient given by the expression (Burken and Schnoor, 1998) $TSCF$ [redacted]$.756e^{\frac{\text{[redacted]}og K_{OW}\text{[redacted]}.50)^2}{2.58}}$, where $\log K_{OI}$ is the logarithm of the octanol-water partition coefficient. The $K_{I,t/.I}$ value was estimated from the octanol-water partition coefficient given by the expression (Trapp et al, 2001) $K_{I\,ul.\,I}$ [redacted]$0^{(\text{[redacted]}\text{[redacted]}\,t!!\,\text{[redacted]}\,l_{ow})}$.

It was supposed that the pesticide degradation rate in the soil solution at the plant rizosphere can be described by a first order kinetic equation given by:

$$C_I(t)\,\text{[redacted]}\,\frac{\text{[redacted]}\,C_I' e^{\text{[redacted]}_s t}}{(\text{[redacted]} f_{OC} K_{OC}\,\text{[redacted]}_I\,\text{[redacted]}_i K_{II})} \tag{2}$$

where C_W^0 [redacted] $\frac{\text{[redacted]}\,C^0_{Soil}}{(f_{OC}\text{[redacted]}K_{OC}\text{[redacted]}_W\text{[redacted]}K_{AW} f_A)}$ (mg l^{-1}) is the soil solution pesticide initial concentration, C^0_{Soil} (mg kg^{-1}) is the pesticide initial concentration in bulk soil, k_s (day^{-1}) is the pesticide dissipation daily rate in the soil, [redacted] (kg l^{-1}) and [redacted] (kg l^{-1}) are the soil densities in a humid basis and dry basis, respectively. K_{AW} is the pesticide air-water partition coefficient. The coefficients f_{OC} (g g^{-1}), f_I and f_i are the soil volumetric fractions of organic carbon, water and air, respectively. The parameter K_{OC} (l kg^{-1}) is the pesticide organic carbon-water partition coefficient and was estimated by the expression (EUSES, 1996) K_{OC} [redacted]$10^{(l.ll\text{[redacted]}\,l_{ow}\text{[redacted]}.ll)}$.

It was supposed that the pesticide initial concentration in the soil solution is known and the one in the plant is null, that is, $C_I(0)$ [redacted]C_I' and $C_{Stem}(0)$ [redacted]. Under these conditions and considering $m_{St}(t)$ [redacted]M[redacted]$_{St}(t)$, the resolution of Eq. (1) that describes the pesticide concentration in the stems is given by:

$$C_{Stem}(t)\,\text{[redacted]}\,\frac{A\,\text{[redacted]}^0_W}{(B\,\text{[redacted]}_s)}[e^{\text{[redacted]}_s t}\,\text{[redacted]}\,\text{[redacted]}^t] \tag{3}$$

where the constants A (l kg^{-1} day^{-1}) and B (day^{-1}) are given by $A \blacksquare \frac{Q \blacksquare TSCF}{M}$ and $B \blacksquare (k_{t} \blacksquare_{G}) \blacksquare \frac{Q}{M \blacksquare K_{\iota\iota\iota,\iota}}$. Constant A is the pesticide uptake rate by plants and constant B is the pesticide dissipation rate from the plant. From Eq. (3) the pesticide concentration in the fruit was estimated by the equation given by:

$$C_{Fruit}(t) \blacksquare \frac{Q_{Phloem} C_{Stem}(t)}{K_{Wood,W}} \blacksquare \frac{A \blacksquare Q_{Phloem} C_{W}^{0} [e^{\blacksquare_{S} t} \blacksquare \blacksquare^{t}]}{K_{Wood,W} (B \blacksquare_{S})} \qquad (4)$$

where $C_{Fruit} \blacksquare C_{Fruit}(t)$ (mg kg^{-1} day^{-1} of fruit fresh mass) is the fruit daily pesticide concentration and Q_{Phloem}(lkg^{-1}) is the volume of water flow in the phloem necessary to produce 1.0 kg of fresh fruit (Trapp et al, 2003). The Eq. (4) allows estimating the time necessary to reach maximum pesticide concentration in fruit and the fruit maximum concentration. The time to reach maximum pesticide concentration in fruit is given by $t_{Fruit}^{Max} \blacksquare \frac{\ln(B) \blacksquare n(k_{s})}{B \blacksquare_{s}}$. And the fruit maximum concentration was calculated by $C_{Fruit}^{Max} \blacksquare C_{Fruit}(t_{Fruit}^{Max})$.

The pesticide bioconcentration in fruit was estimated supposing steady state equilibrium of the quotient between the pesticide concentration in soil solution and in fruits and was calculated by:

$$BCF \blacksquare \lim_{t} \frac{C_{Fruit}(t)}{C_{\iota}(t)} \qquad (5)$$

where BCF (l kg^{-1}) is the pesticide bioconcentration factor in fruit. For the solution of Eq. (1) and to calculate the limit of Eq. (5) it was supposed that the pesticide degradation rate in soil is lower than the pesticide dissipation rate from plant, that is, $k_{\iota} < B$. In this case, the limit for Eq. (5) is given by:

$$BCF = \frac{A \blacksquare Q_{\iota\iota\iota\iota\iota}}{k_{\iota\iota\iota,\iota}(B \blacksquare_{s})} \blacksquare \frac{Q \blacksquare Q_{\iota\iota\iota\iota} \blacksquare TSCF}{Q \blacksquare_{EGS} \blacksquare K_{\iota\iota\iota,\iota} \blacksquare M} \qquad (6)$$

where $k_{EGS} \blacksquare_{E} \blacksquare_{G} \blacksquare_{S}$ (day^{-1}) is the pesticide dissipation rate from the soil-plant system, which allows estimating the half-life time of pesticide dissipation in the soil-plant system, $t_{1/2}$ (day), by the equation $t_{1/2} \blacksquare n(2)/k_{EGS}$.

esults and Discussion

umerical simulation

The pesticide paclobutrazol and a hypothetical mango crop were selected to illustrate the pesticide CF value estimate in fruits using the FTM-p model. In mango orchards, the pesticide paclobutrazol is lso used as growth regulator to control plant growth, maximize mango production, reduce the number of uts and turn easier the orchard cleaning procedures. Soil application of paclobutrazol has been found to more responsive in regard to suppressing the vegetative growth and enhancing the reproductive growth mango than foliar application (Singh, 2000). Sharma and Awasthi (2005) stated that there is an nvironmental contamination risk in areas where paclobutrazol is regularly applied, because this pesticide esidue might persist in the soil for a long period of time. The application of paclobutrazol in the Brazilian ortheastern semi-arid region has become a common practice in commercial mango orchards. The hysical-chemical characteristics (intrinsic properties) of paclobutrazol were obtained from Syracuse esearch Corporation (SRC, 2006) (http://www.syrres.com/esc/physdemo.htm) and are presented in Table

able 1 - Physical-chemical characteristics of paclobutrazol growth regulator used in the FTM-p to imulate the paclobutrazol BCF value in fruits.

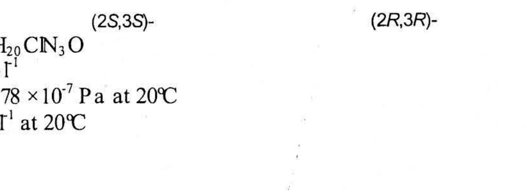
ommon name: paclobutrazol

hemical Abstracts name: *(R*,R*)-(±)-β-[(4-chlorophenyl)methyl]-α-(1,1-dimethylethyl)-1H-1,2,4-iazole-1-ethanol*

AS: 76738-62-0

UPAC name: *(2RS,3RS)-1-(4-chlorophenyl)-4,4-dimethyl-2-(1H-1,2,4-triazol-1-yl)pentan-3-ol*

hemical structure:



(2*S*,3*S*)- (2*R*,3*R*)-

olecular formula: $C_{15}H_{20}ClN_3O$

olar mass: 293.8 g mol^{-1}

apour pressure: 9.999178×10^{-7} Pa at 20°C

Vater solubility: 26 mg l^{-1} at 20°C

${}_{AW}$ [redacted]4.56[redacted]0[redacted]^{0}

og K_{0I} = 3.2

The following assumptions were made to run the FTM-p model: for the estimation of BCF value, n initial paclobutrazol concentration of 1.0 mg kg^{-1} of soil; a five-years-old mango orchard was considered with a total plant dry mass of 6,250.00 kg ha^{-1}, corresponding to 250 plants per hectare, with 25 kg dry mass per plant; transpiration stream was estimated in 20,548.00 l day^{-1} ha^{-1} (750 mm year^{-1} ha^{-1}); plant growth rate was estimated in 2.74[redacted]0^{-5} dia^{-1} (0.01 per year) and a paclobutrazol metabolism rate in mango plants of 0.0462 day^{-1} (the metabolism rate was based on half-life average values of organic compounds in plants estimated by Cousins and Mackay, 2001); the estimated water flow value necessary to produce 1.0 kg of fresh fruit was 5 l kg^{-1}, based on the mango plant water demand increase during fruit development period; the estimated paclobutrazol degradation rate in soil was 0.0073 day^{-1}, corresponding to a half-life of 95 days, experimentally determined in soils from traditional Brazilian mango producing areas (Silva et al. 2003); the paclobutrazol metabolism rate in mango plants and half-life time in soil resulted the dissipation rate in soil-plant system of 0.0389 day^{-1} (k_{EGS}), what corresponded to the dissipation half-life time of 18 days in the soil-plant system.

The soil data used in the simulation were obtained from a Brazilian mango producing semi-arid region, located at the Submédio São Francisco River, close to Petrolina municipal district, State of Pernambuco, Brazil. In general, the mango orchards are established in soils with the following attributes, experimentally determined in soil samples from the 0-0.20 m depth layer (Pessoa, 2003): organic carbon = 0.007 g g^{-1}; volumetric water content at field capacity = 0.15 g g^{-1}; air volumetric content = 0.08 g g^{-1}; soil density in a dry basis = 1.51 kg l^{-1}; soil density in a humid basis = 1.76 kg l^{-1}.

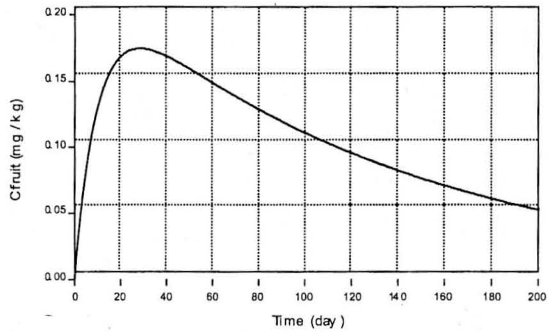
Numerical Results and Discussion

The organic carbon-water partition coefficient value of 492,00 l kg^{-1}, estimated through Eq. (9), indicated that paclobutrazol has moderate affinity with the soil organic matter, what might turn difficult its translocation from soil solution to fruits (Chiou et al, 2001). The value of 4.56×10^{-10} obtained for the air-water partition coefficient, estimated with the data from Table 1, indicated that paclobutrazol is not volatile at room temperature (Trapp and Harland, 1995). The TSCF value of 0.625, estimated through Eq. (3), indicated that paclobutrazol has good mobility in the xylem, what is an important property for plant growth regulators (Lever et al, 1981). The stem-water partition coefficient value of 57,0 l kg^{-1}

$K_{Wood,W}$ [redacted]7,0) indicated that paclobutrazol has a significant affinity with the woody plant material Trapp et al, 2001).

The paclobutrazol concentration in mango fruits (C_{Fruit}) simulated by FTM-p model is illustrated Fig. 1. Initially, fruit concentration is null, increases continuously until a maximum value and after that lecreases with time. This pattern is due to the degradation first order kinetic model supposed for the aclobutrazol concentration in the soil solution (C_{Soil}), to its dissipation rate from the plant (B) and to its ptake rate into the plant (A). At the 27th day (t_{Fruit}^{Max} [redacted]27) after paclobutrazol application to the soil, its oncentration in fruit reaches the simulated maximum value of 0.11 mg kg^{-1}.

The paclobutrazol bioconcentration in the fruit is presented in Fig. 2, and is defined as the quotient etween the concentration in fruit and the concentration in soil solution, $BCF(t)$ [redacted]$_{Fruit}(t)/C_W(t)$. This igure also shows that this quotient equilibrium state is reached for a limit value of 1.87 l kg^{-1}, and this is he paclobutrazol BCF value for the mango fruit. This value can also be obtained directly from Eq. (6).



igure 1 – Paclobutrazol growth regulator concentration in mango fruits simulated by means of FTM-p.

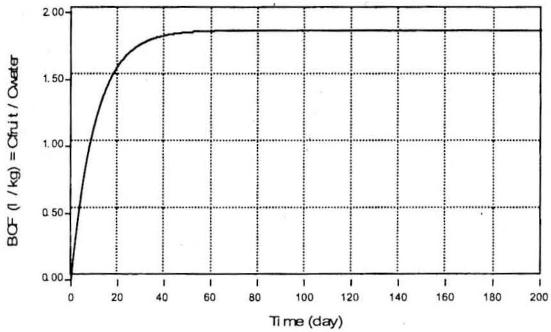


Figure 2 - Paclobutrazol growth regulator bioconcentration factor in mango fruits simulated by means of FTM-p, $BCF(t)$ [redacted] $C_{Fruit}(t)/C_{W}(t)$.

Fig. 2 shows that, initially, the paclobutrazol bioconcentration kinetics in mango fruits is zero, increases continuously following an associative exponential pattern and is limited on the upper part by an asymptote at the level of 1.87 l kg^{-1} parallel to the time axis. Such pattern reaching a plateau at the level of BCF value is a consequence of the fact that the FTM-p model neglects the pesticide transformation processes in the fruit. If the model would incorporate the terms of such processes, the BCF value could be estimated by the quotient between the fruit uptake rate and elimination rate experimentally determined.

Sancho et al (2003) analyzing samples of pears obtained from the fruit market in Spain, did not find any paclobutrazol residues in fruits, but did find paclobutrazol residues at the concentration level of 5.0 µg g^{-1} in pear samples collected from Spanish commercial orchards in which paclobutrazol had been applied to pear trees. Paclobutrazol residues were also found in apple pulp and dry concentrated juice at 12-fold higher levels than in the non-processed fresh juice (IUPAC, 1994). Osuna-García et al (2001) found paclobutrazol traces in Mexican mango fruits (commercial "tommy atkins") treated with paclobutrazol rates during two consecutive years, but did not find any residue when plants were treated in alternated years. In China, Chua et al (2005) also found paclobutrazol residues in commercial apple juices.

FTM-p model sensitivity analysis

Trapp et al (2003) evaluated the FTM model sensitivity as concerned to the entry parameters and concluded that the model is "robust" with respect to plant transpiration and growth rates and stem dry biomass volume. Trapp et al (2003) also agreed that uncertainties in these parameter values do not significantly affect the BCF value in fruits for organic compounds in the range 0.8 [redacted]og K_{ow} [redacted].0. The authors speculated that uncertainties in BCF value might be associated to the xenobiotic metabolic processes in the plant and volatilization.

The sensitivity analysis of FTM-p model can be run directly through Eq. (6), because the pesticide BCF value in fruits is dependent on the water volume in the phloem per 1 kg of fresh fruit (Q_{Phloem}), on the transpiration rate (Q) and on the transpiration stream concentration factor (TSCF). Also, the pesticide BCF value was observed to be inversely dependent to its dissipation rate from the soil-plant system (k_{EGS}), to its plant-water partition coefficient ($K_{Wood/W}$) and to the plant dry biomass (M). Some of the sensitivity analysis results related to the entry data variability are illustrated in Figs. 3 and 4. This analysis was run with the paclobutrazol and mango plant data.

The diagram color bars in Fig. 3 shows the BCF value variability in mango fruits derived from the joint sensitivity analysis of Q and M. This diagram allows inferring that there is no significant variability in paclobutrazol BCF value in mango fruits in consequence of the joint variability of the transpiration rate and dry biomass plant values. There is no significant influence of Q variability on the calculus of paclobutrazol BCF value in mango fruit for the transpiration rate interval usually occurring in adult mango orchards, around 22,000.00 l day^{-1} ha^{-1}. Also, there is no significant influence of mango plant dry biomass variability on the calculus of paclobutrazol BCF value for the M values usually occurring in adult mango orchards, around 6,000.00 kg ha^{-1}. Once known that the volume of water in the phloem stream necessary to produce 1 kg of fresh fruit (Q_{Phloem}) is dependent on Q, it might be also inferred that the variability on Q_{Phloem} values do not significantly affect the paclobutrazol mango fruit BCF values.

The diagram color bars in Fig. 4 shows the pesticide BCF value variability in mango fruits resultant from the joint analysis of pesticide k_{EGS} and logK_{OW}. This diagram shows that no significant variability is observed on the mango fruit pes[redacted]ide BCF values for pesticides with log K_{OW} 1.0 and log K_{OW} [redacted].5 (Fig. 4). However, the same diagram and color bars are indicating there is significant variability on mango fruit pesticide BCF values in function of the variability on pesticide dissipation rate in soil-plant system for pesticides in the range 1.0 [redacted]og K_{OW} [redacted].5 (Fig. 4). This is a consequence of a non-linear relation of TSCF and $K_{Wood,W}$ with log K_{OW} parameters. The optimum pesticide transport from soil to fruits occurs for pesticide with log K_{OW} around 2.2.

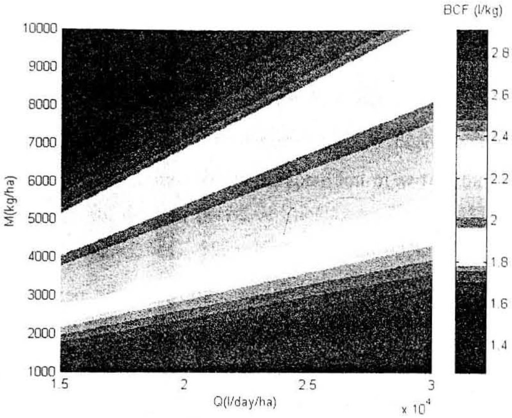


Figure 3 - Diagram representing the joint relation of mango plant dry biomass (M) and transpiration rate (Q) with the paclobutrazol bioconcentration factor (BCF) in mango fruits simulated by means of FTM-p.

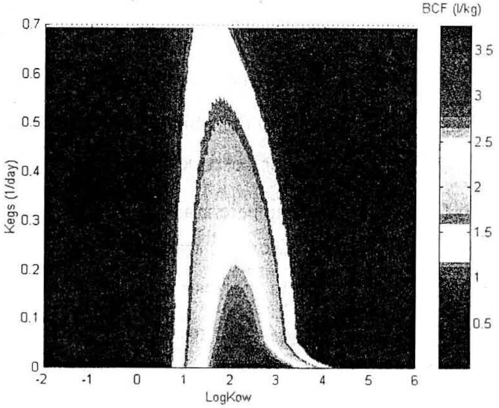


Figure 4 - Diagram representing the joint relation of pesticide octanol-water partition coefficient ($\log K_{OW}$) and the pesticide dissipation rate in the soil-plant system (k_{EGS}) with the pesticide bioconcentration factor (BCF) in mango fruits simulated by means of FTM-p.

Summarizing, the FTM-p model sensitivity analysis shows that the model is "robust" against uncertainties in the physiological parameters values of trees (Q, Q_{Phloem} and M) and to the soil-plant system dissipation rate of pesticides in $\log K_{ow}$ [redacted] and $\log K_{ow}$ [redacted].5 (Fig. 4). Uncertainties in the calculus of mango fruit pesticide BCF value might be associated with uncertainties in the pesticide dissipation and transformation rates in fruits and that were not modeled in this study.

Conclusions

The FTM-p model presented in this work allows estimating the pesticide BCF value in fruits of woody and perennial plants. Pesticides are organic compounds subject to degrading reactions in soils and are taken up by plants from the soil solution through the water transpiration stream. The models FTM and FTM-p are conservative because both hypotheses neglect the pesticide transformation processes in the fruit. Probably, if both models would incorporate the equation terms related to such processes, the BCF value might be calculated as the quotient between the pesticide uptake rate and elimination rate by the fruit. The term added to the FTM model correspondent to the pesticide degradation in the soil, during development of FTM-p model, allowed concluding that pesticide BCF value in mango fruits do not depend on the soil pesticide concentration and on the fresh fruit mass, but is related to the pesticide physical-chemical characteristics (K_{OW}, k_{EGS}) and to the plant physiological parameters (M and Q). The sensitivity analysis of FTM-p model indicates that pesticides with 1.0 [redacted]og K_{ow} [redacted].5 present optimal conditions to bioconcentrate in fruits of woody and perennial plants. And also, that the FTM-p model is "robust" with respect to the plant dry biomass values (M) and water transpiration rate (Q). This analysis also indicates that the model might be sensitive to the pesticide dissipation rate in the soil-plant system (k_{EGS}) for pesticides with 1.0 [redacted]og K_{ow} [redacted].5 (Fig. 4). The results of the sensitivity analysis can be applied to prevent fruit contamination with pesticides with $\log K_{ow}$ around 2.2. Field and laboratory experiments must be carried out in order to validate the use of Eq. (6) presented in this work.

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