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Pesticide bioconcentration modelling for fruit trees

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Abstract

The model presented allows simulating the pesticide concentration evolution in fruit trees and estimating the pesticide bioconcentration factor in fruits. Pesticides are non-ionic organic compounds that are degraded in soils cropped with woody species, fruit trees and other perennials. 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 ($K_{\mathrm{Wood,W}}$), 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 FTM model for pesticides (FTM-p) was applied to a hypothetic mango plant cropping (*Mangifera indica*) treated with paclobutrazol (growth regulator) added to the soil. The model fitness was evaluated through the sensitivity analysis of the pesticide BCF values in fruits with respect to the model entry data variability.

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

1. Introduction

All over the world, fruits are enjoyed for their flavor, color, form and nutritional value and consumed as fresh or processed food. Although tropical regions exhibit privileged climate to cultivate several fruit species, they also provide ideal conditions for the development of weeds, pests and diseases that can economically impair crop production. In general, the fruit tree production management includes the use of pesticides. Brazil is one of the world's greatest fresh-fruit and fruit-juice consumer and exporter and ranks among the world's ten greatest pesticide user (Armas et al., 2005). Therefore, the Brazilian government concern about fruit quality as to fruit pesticide concentration comes with the greatest expectations of Brazilian and foreigner fresh fruit consumers.

Mathematical models might contribute to predict and prevent high toxic substance levels in fruits of orchards treated with pesticides and indicate that such substances must be systematically monitored through good crop management programs. Several mathematical models have been developed to simulate plant uptake of organic substances (Fujisawa et al., 2002; Hung and Mackay, 1997; Matthies and Behrendt, 1995; Paterson and Mackay, 1995; Riederer, 1995; Trapp, 1995; Trapp and Matthies, 1995, 1998; Trapp and McFarlane, 1995; Trapp et al., 2003; Trapp and Pussemier, 1991). Some models were developed to simulate leaf uptake (Trapp and Matthies, 1995), other ones to simulate root uptake (Trapp et al., 2003) and others to simulate both leaf and root uptake (Fujisawa et al., 2002). But, only the model developed by Trapp et al. (2003) aimed at estimating the non-ionic organic compound bioconcentration factor in fruits, taken up by perennial and woody fruit species from soil solution through the transpiration stream and is a steady-state

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fruit-tree model. It considers the stem xylem and phloem transport to fruits.

A substance bioconcentration is defined as the concentration inside and/or on the surface of an organism (or specific tissues) in relation to the substance concentration in the external medium. BCF is a concentration ration at time of harvest. In the chemical equilibrium state, this coefficient is defined as the quotient between the organism and medium substance concentrations. When the organisms are fruit trees and the substance is a pesticide which concentration in the soil solution is known, the fruit BCF value allows estimating the daily pesticide intake through daily fruit intake. Since fruits are the final compartments of several substances taken up by plants from the soil solution, the pesticide BCF value estimate also allows establishing safe limits for the pesticide concentration in the soil solution.

A model that includes the assumption of constant soil pesticide concentration is not adequate to estimate the fruit BCF value, when pesticide is soil-degrading. Therefore, in order to calculate fruit BCF value, the experimental mathematical model is supposed to include a term expressing the soil pesticide degradation; and also, the experiment procedure should avoid transplanting plants to a pesticide-free-medium to calculate the plant pesticide elimination rate. Furthermore, the model is supposed to simulate the pesticide concentration in the soil solution and fruits, in order to use these values to estimate the BCF as the quotient between the fruit and soil solution pesticide concentrations.

This research work aimed at modeling the perennial and woody tree fruit pesticide bioconcentration in order to estimate the fruit pesticide BCF value and the time for maximum fruit pesticide concentration. The BCF equation was based on the pesticide octanol–water partition coefficient, plant transpiration stream, pesticide dissipation rate from the soil–plant system and plant wood biomass. The pesticides considered in this study are soil-degrading non-ionic organic compounds.

2. Material and methods

2.1. Hypothesis for the FTM-p model

The fruit pesticide bioconcentration modeling was developed from the original *Fruit Tree Model* (FTM), according to Trapp et al. (2003), and consisted of adding to it a term that assumes the pesticides are soil-degraded according to a first order kinetic equation. The FTM model was first developed to estimate non-ionic organic compound BCF in fruits under constant soil compound concentrations. In this model, it is assumed that the compound transport from soil to fruit occurs through the plant xylem/phloem flow and is calculated by the solution of a steady state equation expressing the compound mass balance in the soil–plant system.

The modified FTM model, including first order kinetic equations, was named FTM-p (Fruit Tree Model to Pesticide), and then, it was applied to a hypothetical mango (*Mangifera indica*) orchard cultivated with one soil application of paclobutrazol. It is a plant growth regulator taken up into the xylem through the leaves, stems, or roots, and translocated to growing sub-apical meristems. To be applied as a foliar spray, as a soil drench, or by trunk injection (Tomlin, 2000). Paclobutrazol is a plant growth regulator that produces more compact plants and enhances flowering and fruiting.

During the FTM-p modeling, presented below, the original equations and correlations adopted by Trapp et al. (2003) and used to calculate the organic carbon–water partition coefficient (K_{OC}), the transpiration stream concentration factor (TSCF) and the stem-water partition coefficient ($K_{Wood,W}$) were maintained.

The FTM-p modeling assumed that the pesticide dilution processes due to plant growth, plant pesticide metabolism and soil pesticide degradation 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 assumed for woody and perennial fruit trees.

2.2. The FTM-p modeling from FTM model

The pesticide mass balance taken up by plants from soil through the transpiration stream was estimated by the expression (Trapp et al., 2003):

$$\frac{dI_{Xy}}{dt} = QC_{Xy} \tag{1}$$

where: $I_{Xy} = I_{Xy}(t)$ (mg day^{-1} ha^{-1}) is the pesticide mass taken up by plants through the transpiration stream; Q (l day^{-1} ha^{-1}) is the water transpiration rate (transpiration stream) by plants and C_{Xy} (mg l^{-1}) is the pesticide concentration in the transpiration stream.

The transpiration stream pesticide concentration was estimated from the soil solution pesticide concentration and from the pesticide transpiration stream concentration factor, using the expression:

$$C_{Xy} = \text{TSCF}C_W \tag{2}$$

where C_W (mg l^{-1}) is the soil solution pesticide concentration and TSCF is the transpiration stream pesticide concentration factor.

The TSCF value was estimated from the octanol–water partition coefficient given by the expression (Burken and Schnoor, 1998; Trapp et al., 2003):

$$\text{TSCF} = 0.756 \exp\left[\frac{-(\log K_{OW} - 2.50)^2}{2.58}\right] \tag{3}$$

where $\log K_{OW}$ is the logarithm of the octanol–water partition coefficient.