Simulation of the fate of the insecticide carbofuran in a rice field using a level IV fugacity model

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Abstract

The object of this work was to verify the utility of a level IV fugacity model to simulate the environmental fate of the insecticide carbofuran when employed in the cultivation of irrigated rice. The model simulated the dynamic distribution of carbofuran in a system comprising of air, water, rice plants and the soil. The results indicated preferential compartments quality, and provided further knowledge of the fate of carbofuran in rice cultivation. Field experiments on rice were carried out to test the correspondence between simulated and measured carbofuran concentration in water and soil. Simulated concentrations had higher values in the compartments water > soil > rice plants > air. The model can be a useful tool for simulating the environmental fate of this insecticide and can be coupled with sensitivity and uncertainty analyses to test the influence of all input parameters on the outputs.

Additional key words: carbamate, carbosulfan, Oryza sativa, Oryzophagus oryzae, pesticide, weevil.

Resumen

Simulación del comportamiento ambiental del insecticida carbofurano en campos de arroz por el modelo de fugacidad nivel IV

El objetivo de este trabajo fue comprobar la utilidad del modelo de fugacidad nivel IV para simular el comportamiento ambiental del insecticida carbofuran empleado en cultivos de arroz. Con este modelo se simuló la distribución dinámica del carbofurano en un sistema constituido por aire, agua, plantas de arroz y suelo. Los resultados indican los compartimentos preferenciales y permiten predecir el comportamiento ambiental del carbofurano. Para validar el modelo, se realizaron experimentos en campos de arroz verificando la correspondencia entre las concentraciones simuladas y las concentraciones del carbofurano en agua y suelo. Los valores de las concentraciones simuladas en los compartimentos fueron agua > suelo > plantas de arroz > aire. Este modelo puede ser útil para simular el comportamiento ambiental de este insecticida y se puede aplicar el análisis de sensibilidad y de incertidumbre para determinar la influencia de los parámetros de entrada en las salidas del modelo.

Palabras clave adicionales: carbamato, carbosulfano, gorgojo, Oryza sativa, Oryzophagus oryzae, plaguicida.

Introduction

Oryzophagus oryzae (Coleoptera: Curculionidae), commonly known as the rice-infesting weevil, is a major pest of irrigated rice (Oryza sativa) crops. Its larvae cause severe damage to rice roots after flooding and consequently drastically reduce plant nutrient uptake (Carbonari, 2000). When this pest is not controlled grain yield losses may reach 40%. One control procedure is insecticide application, which in recent years has been common in Brazil. Carbofuran has been the most widely used insecticide and the control procedure is the direct application of carbofuran into irrigation water when weevil larvae are detected.

Effectiveness is shown by taking some plants and shaking them into the water, the larvae are visible on the surface of the water (Prando, 2002). Although
carbofuran has good agronomic efficiency, this insecticide has environmental restrictions due to the risk of contamination. A problem frequently associated with carbofuran is the death of forest animals as observed in Virginia by Stinson et al. (1994). Dietrich et al. (1995) reported similar problems for carbofuran granules applied to field crops in Switzerland. Crepeau and Kuivila (2000) suggested the continuous presence of carbofuran in water channels and rivers might cause severe, sub-lethal or chronic damage to aquatic organisms. Gupta (1994) observed carbofuran was toxic to micro crustaceans and vertebrates in the same food chain, and Norberg-King et al. (1991) affirmed that carbofuran was toxic to aquatic wildlife. In 1985, the United States Environmental Protection Agency (EPA) announced a special review of all registered uses of granular carbofuran in the United States because of concerns about its negative impact on birds (James, 1995). Although carbofuran is quickly degraded in the environment, Wayland and Boag (1990, 1995) and Wayland (1991) applied it to prairie wetlands and reported declines in populations of Gammarus lacustris, Chironomus tentans and Hyalella azteca; nymphs of Enallagma genus showed reduced survival. Carbofuran persistence in paddy water and in the soil solution has been studied in tablelands and channels, because carbofuran is mainly degraded by hydrolysis (Seiber et al., 1978; Siddaramappa and Seiber, 1979; Tejada and Magallona, 1985; Jinhe et al., 1989; Mora et al., 1996; Trevizan et al., 2002). However, Chiron et al. (1995) demonstrated that carbamate insecticide concentrations exceeding 0.5 µg L⁻¹, the limit established by the European Community are rarely found in the environment.

Hydrolysis of carbofuran (2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate) in pH range 7-10 is consistent with simple hydrolysis mediated by hydroxyl ions (Seiber et al., 1978). Other factors that might accelerate hydrolysis are high pH (Siddaramappa et al., 1978; Siddaramappa and Seiber, 1979; Chapam and Cole, 1982; Ramanand et al., 1991), the microbial community (Siddaramappa and Seiber, 1979) and light intensity (Seiber et al., 1978; Siddaramappa et al., 1978). Volatilization, photolysis and oxidation are important in carbofuran dissipation (Seiber et al., 1978; Deuel et al., 1979; Mabury and Crosby, 1996). Tejada and Magallona (1985) and Rouchaud et al. (1990) observed that the main carbofuran metabolites are the 3-ketocarbofuran (2,3-dihydro-2,2-dimethyl-3-oxobenzofuran-7-yl methylcarbamate), carbofuran-phenol (2,3-dihydro-2,2-dimethyl-benzofuran-7-ol) and 3-ketocarbofuran-phenol (7-hydroxy-2,2-dimethylbenzofuran-3(2H)-one).

The objective of this work was to verify the utility of a level IV fugacity model to simulate the environmental fate of the insecticide carbofuran in irrigated rice. This fugacity model is a linear system of ordinary differential equations used to estimate fugacities and, hence, the carbofuran concentration in different environmental compartments (i.e. air, water, rice plants and soil). The classification of fugacity models in levels I, II, III and IV is a consequence of the complexity of the calculations and the hypotheses involved in formulation of each level (Mackay, 2001; Paraiba et al., 2002).

### Material and Methods

#### Model development

The relationship between fugacity and concentration is given by:

\[ C = Z_f \]  

where \( C \) (mol m⁻³) is the pesticide concentration, \( f \) (Pa) is the pesticide fugacity and \( Z \) (mol m⁻³ Pa⁻¹) is the fugacity capacity. The fugacity capacity depends on the compartment and on the pesticide physical-chemical properties. Thus, due to the proportionality between \( C \) and \( Z \), compartments with high fugacity capacities for a pesticide will also have high pesticide concentrations. The compartments of the rice cultivation system modelled in this work are air \((i = a)\), water \((i = w)\), rice plants \((i = r)\) and soil \((i = s)\), \( i \in I = \{a, w, r, s\} \).

The pesticide partition coefficient, \( k_{ij} \), between the compartments \( i \) and \( j \) is defined as:

\[ k_{ij} = \frac{C_i}{C_j} \]  

where \( C_i \) and \( C_j \) are the pesticide concentrations of compartments \( i \) and \( j \) in identical volumetric units such as mol m⁻³, respectively. When \( f_i = f_j \) the partition coefficient \( k_{ij} \) is determined by:

\[ k_{ij} = \frac{Z_i}{Z_j} \]  

where \( Z_i \) and \( Z_j \) are the fugacity capacities of compartments \( i \) and \( j \), respectively.
The fugacity capacity of air \((Z_a)\) is defined by:
\[
Z_a = \frac{1}{RT}
\]
[4]
where \(T(K)\) is the air temperature and \(R\) (8.314 m\(^3\) Pa mol\(^{-1}\) K\(^{-1}\)) is the gas constant. The fugacity capacity of water \((Z_w)\) is defined by:
\[
Z_w = \frac{1}{H} + \frac{oc_w \rho_w k_{oc}}{H}
\]
[5]
where \(H\) (m\(^3\) Pa mol\(^{-1}\)) is Henry's constant of the pesticide, \(oc_w\) (m\(^3\) m\(^{-3}\)) is the organic carbon volumetric fraction of the water, \(\rho_w\) (kg m\(^{-3}\)) is the water density (999.5 kg m\(^{-3}\)) and \(k_{oc}\) (m\(^3\) kg\(^{-1}\)) is the organic carbon partition coefficient of the pesticide. Henry's constant was estimated by:
\[
H = \frac{p_m p_v}{w_v}
\]
[6]
where \(p_m\) (g mol\(^{-1}\)) is the pesticide molar mass, \(p_v\) (Pa) is the pesticide vapor pressure and \(w_v\) (g m\(^{-3}\)) is the pesticide aqueous solubility. The fugacity capacity of the rice plants \((Z_r)\) was estimated by:
\[
Z_r = (x_w Z_w + x_l k_{lw} Z_w) \rho_r/\rho_w
\]
[7]
where \(\rho_r\) (kg m\(^{-3}\)) is the rice plant density, \(k_{lw}\) (m\(^3\) m\(^{-3}\)) is the pesticide octanol-water partition coefficient, \(x_w\) (m\(^3\) m\(^{-3}\)) is the water volumetric fraction of the rice plant and \(x_l\) (m\(^3\) m\(^{-3}\)) is the volumetric fraction of lipids of the rice plant (Trapp and McFarlane, 1995; Cousins and Mackay, 2001). The fugacity capacity of the soil \((Z_s)\) was estimated by:
\[
Z_s = \frac{\theta}{H} + \frac{oc_s \rho_s k_{oc}}{H}
\]
[8]
where \(\theta\) (m\(^3\) m\(^{-3}\)) is the water volumetric fraction of the soil, \(\rho_s\) (kg m\(^{-3}\)) is the density of soil, \(oc_s\) (m\(^3\) m\(^{-3}\)) is the organic carbon volumetric fraction of the soil and \(k_{oc}\) (m\(^3\) kg\(^{-1}\)) is the organic carbon partition coefficient of the pesticide (Mackay et al., 1996).

Pesticide mass flow resulting from diffusion between two contiguous compartments \(i\) and \(j\), \(N_{ij}\) (mol h\(^{-1}\)), can be calculated by:
\[
N_{ij} = d_{ij} (f_i - f_j)
\]
[9]
where \(d_{ij}\) (mol Pa\(^{-1}\) h\(^{-1}\)) is the transfer coefficient. According to Fick's first law, these transfer coefficients are given by:
\[
d_{ij} = \frac{A_{ij} D_{pi} D_{pj} Z_i Z_j}{\delta_{ij} (D_{pi} Z_i + D_{pj} Z_j)}
\]
[10]
where \(A_{ij}\) (m\(^2\)) is the contact area between compartments \(i\) and \(j\), \(D_{pi}\) (m\(^2\) h\(^{-1}\)) is the pesticide diffusivity in compartment \(i\), \(D_{pj}\) (m\(^2\) h\(^{-1}\)) is the pesticide diffusivity in compartment \(j\), \(\delta_{ij}\) (m) is the thickness of the diffusion layer between compartments \(i\) and \(j\) (Zitko and McLeese, 1980).

The water and soil contact areas between the 0.0-0.2 m depth was calculated by the expression:
\[
A_{ws} = \rho_s S V_s
\]
[11]
where \(S_s\) (m\(^2\) kg\(^{-1}\)) is the soil specific surface area. The value of \(S_s\) was estimated by the relationship:
\[
S_s = 10^3 (1313.78 oc_s + 117.00 c_l + 116.90 s_t + 5.15 s_d)
\]
[12]
where \(c_l\) (m\(^3\) m\(^{-3}\)) is the clay volumetric fraction of the soil, \(s_t\) (m\(^3\) m\(^{-3}\)) is the silt volumetric fraction of the silt and \(s_d\) (m\(^3\) m\(^{-3}\)) is the sand volumetric fraction of the soil (Paraiba et al., 2004).

Pesticide diffusivity in air \(D_{pa}\) (m\(^2\) h\(^{-1}\)) was estimated by:
\[
D_{pa} = \frac{3.6 \times 10^{-4} T^{1.75} \sqrt{M_{pa}}}{(3N_p + 3N_a)}
\]
[13]
where \(N_p\) (cm\(^3\) mol\(^{-1}\)) is the molar volume of the pesticide, \(N_a\) (cm\(^3\) mol\(^{-1}\)) is the molar volume of the air (20.0 cm\(^3\) mol\(^{-1}\)) and \(M_{pa}\) is given by:
\[
M_{pa} = \frac{p_m + a_m}{p_m p_a}
\]
[14]
where \(a_m\) (g mol\(^{-1}\)) is the molar mass of air (28.9 g mol\(^{-1}\)) (Lyman et al., 1990). Pesticide diffusivity in water, \(D_{pw}\) (m\(^2\) h\(^{-1}\)), was estimated by:
\[
D_{pw} = \frac{2.056 \times 10^{-7} T \phi_{w_m}^{0.6}}{\mu_w (V_p)^{0.6}}
\]
[15]
where \(\phi_{w_m}(2.6)\) is an association term for the water, \(w_m\) (18 g mol\(^{-1}\)) is the molar mass of water and \(\mu_w\) (8.9 \times 10\(^{-1}\) centipoises) is the water viscosity (Weber and DiGiano, 1996). Considering that rice plants have a high water volumetric fraction (> 0.8 m\(^3\) m\(^{-3}\)), the model supposes that the diffusivity of the pesticide in rice plants is equal
to the diffusivity of the pesticide in water \((D_{pw} = D_{pw})\). Pesticide diffusivity in soil \(D_{ps}\) \((m^2 \cdot h^{-1})\) can be estimated by:

\[
D_{ps} = \frac{D_{pw} \varphi_s^2}{(1 - \varphi_s) \rho_s oc k_{oc} \varphi_s + \varphi_s} \tag{16}
\]

where \(\varphi_s\) \((m^3 \cdot m^{-3})\) is the soil porosity (Wu and Gschwend, 1986).

Pesticide disappearance or transformation in air, water, rice plants and the soil can occur by physical and chemical process, by biological degradations, by dilution during rice growth or by water volume variation in rice fields. These pesticide processes are assumed to be first-order and are described by:

\[
\frac{dC_i}{dt} = -\lambda_i C_i \tag{17}
\]

where \(\lambda_i\) \((h^{-1})\) is the transformation rate which was estimated by:

\[
\lambda_i = \frac{\ln 2}{t_{1/2}} \tag{18}
\]

where \(t_{1/2}\) \((h)\) is the pesticide half-life in compartment \(i \in I = \{a, w, r, s\}\). Thus, in a level IV fugacity model the term that describes pesticide transformation or disappearance in a compartment \(i\) is given by:

\[
\frac{df_i}{dt} = -\lambda_i f_i V_i Z_i \tag{19}
\]

where \(V_i\) \((m^3)\) is the volume of compartment \(i\).

Pesticide advection in compartment \(i\) can be introduced into the model as a first-order process. In fact, advection can be regarded as a constant speed, defined as the algebraic sum between the entry flow \(G_i C_{Bi}\) and the exit flow \(G_i f_i\), where \(G_i\) \((m^3 \cdot h^{-1})\) is the matter flow \(i\) entering compartment \(j\) with concentration \(C_{Bi}\) and leaving this compartment with concentration \(C_i\) (Mackay, 2001).

It is assumed that direct transfer of pesticide mass occurs from the air to water and rice plants, from water to air, soil and rice plants, from rice plants to air and water and from soil to water. Thus, the mass distribution of the pesticide is given by a system of ordinary differential equations:

\[
\frac{df_i}{dt} = \frac{N_{aw}}{V_i Z_i} + \frac{N_{ew}}{V_i Z_i} + \frac{N_{sw}}{V_i Z_i} + \frac{G_i C_{Bi}}{V_i Z_i} - \frac{G_i f_i}{V_i Z_i} - \lambda_i f_i \tag{20}
\]

The observed soil concentration was estimated from the observed soil solution concentration using the equation given by:

\[
f_t = \frac{oc p_k \rho_{skoc}}{p_m} C_{ss} \tag{25}
\]

where \(C_{ss}\) \((mg \cdot L^{-1})\) is the observed soil solution concentration of carbofuran.

**Field experiment and input dates**

A field experiment was carried out on 200 ha of irrigated rice crop located in Bariri municipality, State of São Paulo, Brazil \((22° 02' 45'' S\) and \(48° 43' 46'' W\) altitude 450 m). The area was subdivided in 1.5 and 2.5 ha rice fields that were separated by irrigation and drainage channels. The experimental unit was 2 ha and was located at the first water entry to avoid contamination. Soil is classified as a Gleissolos (Oliveira et al., 1999). Soil samples, collected before the start of the experiment, did not contain carbofuran. The area was managed according to the usual procedures for an irrigated rice crop. There was a pre-sowing irrigation to induce germination of red rice and other weeds. The area was flooded and drained. After weed emergence the following herbicides were applied: glyphosate at 3.3 L ha\(^{-1}\) and 2,4-D at 0.75 L ha\(^{-1}\) (Foloni, 1999). Twenty-two days after post-emergence weed control \(22\) November 2002), rice cv IRG 420 was seeded with a NPK fertilizer of \(05-25-25\) at 250 kg ha\(^{-1}\). One day after sowing clomazone was applied at 0.66 L ha\(^{-1}\). Following that the filed was irrigated by fast flooding and drained to inducing seed germination. Fifteen days after seedling emergence,
the area was flooded again and this water was maintained in the field until the day before harvest. A dressing of nitrogen was applied as urea at 27 and 45 d after sowing at 50 and 80 kg ha\(^{-1}\), respectively. Before application of the carbofuran the water layer was maintained on the field for 48 h. The crop was harvested 105 days after sowing.

**Soil solution and water sampling**

The soil solution sampler was a porous capsule attached to a PVC tube (1.27 cm inner diameter and 30 cm long), two silicone corks (one in a plastic bottle and the other in the PVC tube) and a hose. The soil solution was pumped through the hose to the bottle with a manual pump. When the soil was dry, 8 samplers were randomly installed in the experimental area at 20 cm depth, 9 days before rice sowing. Laminar water flow was also collected using plastic bottles. Samples were obtained by fast bottle immersion at 8 randomly selected places in the plot. Temperature and pH were determined for all laminar water and soil solution samples using a portable pH-meter (PG1400, GENAKA). Samples were immediately placed in an icebox for transportation and were stored at –18°C. Laminar water and soil solution were sampled at 24, 48, 96, 192, 384 and 768 hours after carbofuran application.

**Analytical procedure**

All samples were stored at –18°C for five months prior to laboratory analysis. Carbofuran extraction from water consisted of a 100 ml sample extraction of dichloromethane (Leppert et al., 1983). Carbofuran was measured using a gas chromatography system HP-5MS capilar column (length - 30 m, diameter - 0.25 mm); (film thickness - 0.25 µm), with the oven temperature programmed as follows: initial = 100°C, for 1 min; slope: 25°C up to 280°C, kept for 2.5 min. A mass selective detector (MSD) was coupled to the chromatograph, which was operated in the ion monitoring system (SIM), analysing a single fragment (fragment 160) for carbofuran measurements.

**Carbofuran physicochemical properties and input dates**

The carbofuran physicochemical characteristics required for the study and the simulation of insecticides behaviour and environmental fate by a level IV fugacity model are presented in Table 1. Carbofuran was applied at 1.05 \(\times\) 10\(^{-4}\) mol m\(^{-2}\) (0.23 kg ha\(^{-1}\)) that gave a concentration of 1.04 \(\times\) 10\(^{-3}\) mol m\(^{-3}\) (0.2301 mg L\(^{-1}\)) in the water at 24 h after application. This fell to 3.67 \(\times\) 10\(^{-6}\) mol m\(^{-3}\) (8.1 \(\times\) 10\(^{-4}\) mg L\(^{-1}\)) at 768 h after application.

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Common name(^1)</td>
<td>Carbofuran</td>
</tr>
<tr>
<td>CAS(^1)</td>
<td>1563-66-2</td>
</tr>
<tr>
<td>Class(^1)</td>
<td>Carbamate</td>
</tr>
<tr>
<td>Agronomic function(^1)</td>
<td>Insecticide and nematicide</td>
</tr>
<tr>
<td>Chemical abstract name(^1)</td>
<td>2,3-dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate</td>
</tr>
<tr>
<td>IUPAC name(^1)</td>
<td>2,3-dihydro-2,2-dimethylbenzofuran-7-yl methylcarbamate</td>
</tr>
<tr>
<td>Chemical structure(^1)</td>
<td></td>
</tr>
<tr>
<td>Formulae molecular(^1)</td>
<td>C(<em>{12})H(</em>{15})NO(_3)</td>
</tr>
<tr>
<td>Molar mass(^1)</td>
<td>221.3 g mol(^{-1})</td>
</tr>
<tr>
<td>Molar volume(^2)</td>
<td>194.4 cm(^3) mol(^{-1})</td>
</tr>
<tr>
<td>Vapor pressure(^1)</td>
<td>3.1 (\times) 10(^{-4}) Pa (20°C)</td>
</tr>
<tr>
<td>Water solubility(^1)</td>
<td>351 mg L(^{-1}) (20°C)</td>
</tr>
<tr>
<td>log (k_{ow})(^1)</td>
<td>1.52 (20°C)</td>
</tr>
<tr>
<td>(k_{oc})(^3)</td>
<td>0.022 m(^3) kg(^{-1})</td>
</tr>
</tbody>
</table>

Numerical simulation and input dates

Carbofuran half-lifes in water and in soil solution were estimated as 78 and 241 h, respectively (Plese et al., 2005). Carbofuran half-life in air and rice plants was determined as 12 h and 36 h, respectively (Tejada and Magallona, 1985). These measured carbofuran half-life values for soil, water, air and rice plants were used as the input values for the numerical simulations.

The thickness of the diffusion layer between contiguous compartments was selected as 1.0 × 10⁻⁴ m (Zitko and Mc Leese, 1980). Soil density, porosity, and organic carbon, clay, silt and sand volumetric fraction were measured using site-specific soil samples and had values of 1.54 × 10³ kg m⁻³, 0.42, 0.017, 0.25, 0.09 and 0.64 m³ m⁻³, respectively. The organic carbon volumetric fraction of the water was 1.2 × 10⁻¹ m³ m⁻³. The average volumetric fraction of water in soil was 0.48 m³ m⁻³ at 0-0.2 m depth. The specific surface area of the soil was estimated as 78 and 241 h, respectively (Plese et al., 2005). Carbofuran half-life in air and rice plants was estimated as 12 h and 36 h, respectively (Tejada and Magallona, 1985). These measured carbocuran half-life values for soil, water, air and rice plants were used as the input values for the numerical simulations.

The transfer coefficients between air and water, water and soil, air and rice plants, and water and rice plants were estimated as 2.0 × 10⁴, 4.03 × 10¹¹ [Eq. 11], 1.5 × 10⁴, and 3.0 × 10³ m², respectively.

The density of the rice plants, volumetric fraction of water and lipids in rice plants were 1.03 × 10³ kg m⁻³, 0.80 and 0.02, respectively. The average air temperature was 298°K. For i, j ∈ I the model supposes that dij = dji and diw = dw. Volumes of air, water, rice plants and soil were 8.0 × 10⁴, 2.0 × 10⁵, 1.2 × 10⁵, and 5.0 × 10⁵ m³, respectively.

The calculated fugacity capacities of the air, water, soil, rice plants and air and rice plants and water and rice plants were 1.89 × 10⁶, 2.2 × 10⁶, 3.3 × 10⁴ and 3.8 × 10⁴ mol m⁻³ Pa⁻¹, respectively. The calculated carbofuran air-water partition coefficient was 1.83 × 10⁻⁸ [Eq. 3]. Pesticides with kaw ≤ 4.0 × 10⁻⁴ are not volatile under atmospheric temperatures (Trapp and Harland, 1995). As a result carbofuran does not volatilize under normal atmospheric temperatures. The calculated carbofuran rice-water partition coefficients was 1.52 [Eq. 3]. These partition coefficients partially explain the simulated concentration levels in the rice plants. Soil sorption and soil-water partition coefficient of carbofuran, kw = 0.022 m³ kg⁻¹ and kaw = 1.75 [Eq. 3], respectively, indicate a low affinity with soil solid particles and a high affinity with both laminar water and the soil solution.

Results and Discussion

The simulations showed that the time required for the fugacity values to stay within a range of a final equilibrium value is over 1,000 h. It is after this time has elapsed that there should be an analysis of the distribution of carbofuran in air, water, rice plants and soil using a steady state fugacity model type (level I, II or III fugacity model). Fugacity decreases uniformly in all compartments until it reaches equilibrium with fugacity values around 10⁻¹² Pa [Eqs. 20-23]. Carbofuran concentration decreases in water while it increases in air, rice plants and soil up to a maximum and then decreases (Figs. 1-2). The main reasons for carbofuran behaviour in these environmental compartments can be explained by its properties such as high water solubility, low vapour pressure, low soil-water partition coefficient and a low octanol-water partition coefficient that lead to high affinity to water (simulated and measured) and rice plants (simulated). Carbofuran concentration showed higher values in the following compartments: water > soil > rice plants > air. In general, carbofuran is only applied to water and it is then transferred to rice plants and soil.

The calculated fugacity capacities of the air, water, rice plants and soil were 4.04 × 10⁴, 2.2 × 10⁴, 3.3 × 10⁴ and 3.8 × 10⁴ mol m⁻³ Pa⁻¹, respectively. The calculated carbofuran air-water partition coefficient was 1.83 × 10⁻⁸ [Eq. 3]. Pesticides with kaw ≤ 4.0 × 10⁻⁴ are not volatile under atmospheric temperatures (Trapp and Harland, 1995). As a result carbofuran does not volatilize under normal atmospheric temperatures. The calculated carbofuran rice-water partition coefficients was 1.52 [Eq. 3]. These partition coefficients partially explain the simulated concentration levels in the rice plants. Soil sorption and soil-water partition coefficient of carbofuran, kw = 0.022 m³ kg⁻¹ and kaw = 1.75 [Eq. 3], respectively, indicate a low affinity with soil solid particles and a high affinity with both laminar water and the soil solution.

Figure 1. Carbofuran concentrations in air (● 1.0E + 6 × Cₐ) and in rice plants (○ Cₚ) as simulated by a level IV fugacity model.
The level IV fugacity models used here underestimated the water carbofuran concentrations and partially underestimated the soil carbofuran concentrations \((t < 120 \text{ h})\) (Fig. 2). This can be associated with the definition assumed of the fugacity capacity of the water and soil, and the carbofuran half-life in water and soil used in this work. A level IV fugacity model can reasonably predict carbofuran concentration in the rice growing environment. As the carbofuran concentrations was not measured in air and rice plants no conclusions were drawn concerning predictions of carbofuran concentration in these two compartments. Generally, the level IV fugacity model used in this study have shown a good possibility for use as a tool to predict the fate of organic chemicals in different environmental compartments. The results suggest that the model could be used to determine which environmental compartment was more vulnerable to carbofuran. Generally the results suggest that the model is appropriate and can be used to estimate carbofuran fate and exposure in an environmental compartments system for screening for risk analysis. The level IV fugacity model can be considered a useful tool for simulating the environmental fate of this insecticide and could be coupled with sensitivity and uncertainty analyses to test the influence of all input parameters and make assumptions on the outputs.

**Acknowledgements**

The authors thanks Mr Reinaldo Belluzo Foloni for field assistance in the Varjão Farm, Bariri City, and State of São Paulo. This study was funded by Fundo de Apoio ao Ensino e a Pesquisa (FAEP) of Universidade Estadual de Campinas (UNICAMP), CAPES/MEC (Brazil), EMBRAPA/PRODETAB (Brazil) and MCYT (Spain) (AGL2002-04532-C03) grant to authors.

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