Application of System Dynamics technique to simulate the fate of persistent organic pollutants in soils

R. Chaves [a,*], D. López [b], F. Macías [a], J. Casares [b], C. Monterroso [a]

[a] Departamento de Edafoloxía e Química Agrícola, Facultade de Bioloxía, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain
[b] Departamento de Enxeñaría Química, ETSE, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain

HIGHLIGHTS

► We construct a model to simulate the behavior of pop's in contaminated soils.
► We use the technique of System Dynamics to solve the model.
► We obtain the contribution of each pathway to remove the lindane in soil.
► Infiltration and biochemical degradation pathways are more decisive.
► The model is highly sensitive to the half-life of lindane, highly uncertain value.

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ABSTRACT

Persistent organic pollutants (POPs) are within the most dangerous pollutants released into the environment by human activities. Due to their resistance to degradation (chemical, biological or photolytic), it is critical to assess the fate and environmental hazards of the exchange of POPs between different environmental media.

System Dynamics enables to represent complex systems and analyze their dynamic behavior. It provides a highly visual representation of the structure of the system and the existing relationships between the several parameters and variables, facilitating the understanding of the behavior of the system. In the present study the fate of γ-hexachlorocyclohexane (lindane) in a contaminated soil was modeled using the Vensim® simulation software.

Results show a gradual decrease in the lindane content in the soil during a simulation period of 10 years. The most important route affecting the concentrations of the contaminant was the biochemical degradation, followed by infiltration and hydrodynamic dispersion. The model appeared to be highly sensitive to the half-life of the pollutant, which value depends on environmental conditions and directly affects the biochemical degradation.

1. Introduction

Organochlorine pesticides (OCPs) are persistent organic pollutants (POPs) that have been identified in diverse environmental matrices worldwide. Soils are an important sink for POPs, especially for OCPs, due to their low solubility and volatility, and their strong sorption by soil organic matter (Zhang et al., 2011). One of commonly used OCPs in agriculture was γ-hexachlorocyclohexane (lindane), now obsolete.

To simulate the fate of pesticides in the environment mathematical models have been developed (Koziol and Pudykiewicz, 2001; Li et al., 2002; Ao et al., 2009). Models that simulate the

movement of pesticides in soil are complex and take into account diverse processes, including leaching, adsorption, degradation, surface run-off, uptake by plants and volatilization (Chu and Mariño, 2007; Köhne et al., 2009). Moreover, numerical resolution of these models involves a great effort due to the mathematical complexity and the required programming knowledge. In this respect, visual modeling based on System Dynamics has greatly improved the accessibility of such modeling tools (Muetzelfeldt and Massheder, 2003).

System Dynamics was designed to understand complex models and to assess the relations between the structure of a system and its behavior over time (Ford, 2009). The technique formulates a system in terms of ordinary differential equations (ODEs), representing it graphically by simple blocks of stocks and flows that form feedback loops. The development of user-friendly software

(e.g. Dynamo, Stella, PowerSim, Vensim) has popularized these modeling techniques in numerous fields of research (Ford, 2009).

The objective of the present research was to understand the behavior of a persistent organic pollutant in soil–plant system, evaluating critical routes and parameters in the dissipation of the pollutant. System Dynamics was chosen for this purpose and the model was implemented in Vensim® software (Ventana Systems, 2007) due to its performance and handy use, prior to design a real assay, saving time and money.

2. Methodology

2.1. Description of the conceptual model

This work was based on a unidimensional model developed by Chu and Mariño (2004) for the vadose zone that assumes vertical flow throughout the soil profile. The conceptual model was structured by dividing the soil profile into three zones: surface-, root-, and deep-zone (Fig. 1).

The model consider the following processes: (a) advection, i.e. passive movement of solutes dissolved in water; (b) diffusion or movement of molecules due to the existence of concentration gradients; (c) dispersion, derived from variations in speed of flow within a porous medium; (d) adsorption, or accumulation of the compound at the interface between a solid surface and the solution; (e) degradation, or rupture of the molecular structure of the contaminant; (f) volatilization, or transfer of the contaminant to the vapor phase; and (g) root uptake, which is affected by evapotranspiration.

2.2. Mathematical expression of contaminant fate

The mathematical expressions is based on the resolution of a system of coupled differential equations that describe the movement of water in a porous medium (governed by the equation of Richards), and the movement of the contaminant (governed by the advective–dispersive transport model). The variation of the concentration of pollutant considers therefore transport phenomena, but also other removal processes, such as biochemical degradation of the pollutant or root uptake.

The model proposed by Chu and Mariño (2004) assumes the following: (a) theoretical complete mixing of the solute; (b) transport under isothermic conditions; (c) linear equilibrium in the process of adsorption–desorption of the contaminant; (d) linear liquid–vapor distribution coefficient, based on Henry's law; and (e) first order degradation constant for the contaminant. The concentration varies not only with time, but also with space, resulting in a PDE (partial differential equations) model.
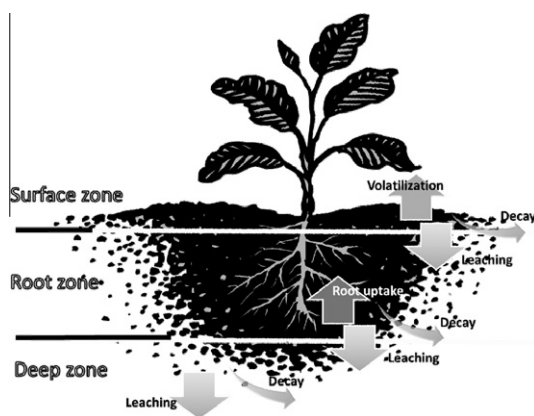

Fig. 1. Conceptual model of pollutant fate in soil.

The mathematical expression of the model is as follows:

$$\frac{\partial C}{\partial t} = \frac{1}{\theta + \rho K_d + aK_H} \left\{ \frac{\partial}{\partial z}\left[aD_g\frac{\partial(K_H C)}{\partial z}\right] + \frac{\partial}{\partial z}\left[\theta D_l \frac{\partial C}{\partial z}\right] \right.$$
$$\left. - \frac{\partial(qC)}{\partial z} - FS \cdot C - \frac{aD_g^a K_H}{d \cdot z_v}C - (\theta + \rho K_d + aK_H)k_sC + M(z,t) \right\} \quad (1)$$

C = concentration of contaminant in the soil solution $[ML^{-3}]$; θ = volumetric water content of the soil $[L^3L^{-3}]$; a = volumetric air content of the soil $[L^3L^{-3}]$; ρ = apparent density of the soil $[ML^{-3}]$; K_d = distribution coefficient $[L^3M^{-1}]$; K_H = Henry's constant (dimensionless); D_g = coefficient of diffusion of the contaminant in the vapor phase $[L^2T^{-1}]$; D_l = coefficient of dispersion of the contaminant in the dissolved phase $[L^2T^{-1}]$; D_g^a = coefficient of diffusion of the vapor phase of the contaminant in the open air $[L^2T^{-1}]$; q = water flow or mean velocity of flow $[L\ T^{-1}]$; k_s = first order degradation constant for the contaminant $[T^{-1}]$; d = thickness of the layer bounded by the air $[L]$, for which the value suggested by Jury et al. (1991), 5 mm, was used; z_v = depth of the surface layer considered for the volatilization, $[L]$; S = water uptake rate by the plant $[L^3L^{-3}T^{-1}]$; F = concentration factor for the transpiration flow (dimensionless); and $M(z, t)$ = loading term or input of contaminant $[ML^{-3}T^{-1}]$.

The model proposed by Chu and Mariño (2004) was completed in present study introducing the influence of organic matter content of soils on both the distribution coefficient (K_d) and the soil density (ρ). This enabled a better adaptation of the model to assess the behavior of OCPs in different types of soils (Section 3.2.).

2.3. Model construction with Vensim® software and mathematical resolution

In order to assimilate Eq. (1) to a System Dynamics model, the derivatives were reformulated with respect to the space by numerical approximation, leaving the model derivated just with respect to the time. Each layer of soil profile was represented by stock variable of its pollutant concentration in the dissolved phase, with different flows entering or leaving as represented in Fig. 1.

The gradients and secondary derivatives with respect to the space, which vary dynamically as the model is resolved, were reformulated by means of a Taylor series truncated at the 2nd term. Substituting the space derivatives from Eq. (1) with a Taylor series approximation, and considering that all the parameters remain constant in each layer, the resulting differential equation is:

$$\frac{\partial C}{\partial t} = \frac{1}{\theta + \rho K_d + aK_H}\left[aD_g K_H\frac{C(z+h) - 2C(z) + C(z-h)}{(\Delta z/2)^2} \right.$$
$$+ \theta D_1\frac{C(z+h) - 2C(z) + C(z-h)}{(\Delta z/2)^2} - q\frac{C(z+h) - C(z-h)}{\Delta z}$$
$$\left. - FS \cdot C - \frac{aD_g^a K_H}{d \cdot \Delta z_v}C - (\theta + \rho K_d + aK_H)k_sC + M(z,t) \right] \quad (2)$$

For greater simplicity for the graphical representation of the model in Vensim®, the parameters were grouped as follows:

$$R = \theta + \rho K_d + aK_H \quad (3)$$

$$ELV = \frac{aD_g K_H}{(\Delta z/2)^2} \quad (4)$$

$$ESL = \frac{\theta D_l}{(\Delta z/2)^2} \quad (5)$$

R is the retardation factor, ELV represents the liquid–vapor equilibrium of pollutant, and ESL the liquid–solid equilibrium. Substituting the previous groups of variables in Eq. (2), we obtain the equation that was used to implement the model in Vensim®:

$$\frac{\partial C}{\partial t} = \left[\frac{ELV}{R} \frac{C(z+h) - 2C(z) + C(z-h)}{(\Delta z/2)^2} + \frac{ESL}{R} \frac{C(z+h) - 2C(z) + C(z-h)}{(\Delta z/2)^2} - \frac{q}{R} \frac{C(z+h) - C(z-h)}{\Delta z} - \frac{FS}{R} \cdot C - \frac{aD_g^a K_H}{R \cdot d \cdot \Delta z_v} C - k_s C + \frac{M(z,t)}{R} \right]$$

(6)

Eq. (6) represents several transport phenomena and routes of pollutant exchange between different media, as shown in following equations:

$$evapor = \frac{ELV}{R} \frac{C(z+h) - 2C(z) + C(z-h)}{(\Delta z/2)^2} \quad (7)$$

$$disp = \frac{ESL}{R} \frac{C(z+h) - 2C(z) + C(z-h)}{(\Delta z/2)^2} \quad (8)$$

$$flow = \frac{q}{R} \frac{C(z+h) - C(z-h)}{\Delta z} \quad (9)$$

$$rootuptake = \frac{FS}{R} \cdot C \quad (10)$$

$$volat = \frac{aD_a K_H}{R \cdot d \cdot \Delta z_v} C \quad (11)$$

$$decaydis = k_s C \quad (12)$$

$$load = \frac{M(z,t)}{R} \quad (13)$$

Eq. (6) was adapted, considering the processes present on each layer:

Surfacezone:

$$\frac{\partial(Csurf)}{\partial t} = [evaporsurf + dispsurf + load - flowsurf - volat - decaydissurf] \quad (14)$$

Rootzone:

$$\frac{\partial(Croots)}{\partial t} = [evaporroots + disproots + flowsurf - flowroots - rootuptake - decaydisroots] \quad (15)$$

Deepzone:

$$\frac{\partial(Cdeep)}{\partial t} = [evapordeep + dispdeep + flowroots - flowdeep - decaydisdeep] \quad (16)$$

In order to apply the Taylor series, for each iteration n, three values of the concentration of pollutant for each layer need to be known from iteration $n - 1$: $C(z - h)$, $C(z)$ and $C(z + h)$. $C(z)$ was assumed to be the value of the stock of each layer, whereas the superior $C(z - h)$ and inferior $C(z + h)$ values were approximated as a weighted interpolation of the concentrations of the neighbor layers. The top and bottom boundary concentrations were also calculated by extrapolation of the concentration of lindane in the surface and deep zones, given the existing linear relation for the concentrations of the three layers, which appeared to be maintained during the period of simulation. Detailed information is available in the Supplementary Material.

A diagram of the model constructed with the Vensim® software (Fig. 2) shows the three stocks: Csurf (dissolvsurf), Croots (dissolvroots) and Cdeep (dissolvdeep), with their associated inputs and outputs as expressed by Eqs. (14)–(16), and the different model parameters involved in the model. The load term (13) was considered zero since no source is adding new pesticide to the soil.

3. Application

3.1. Study area

The simulation study was carried out in a level experimental plot with a surface area of 3700 m² , located in a site contaminated by waste generated by lindane production in O Porriño (NW Spain). The climate is mild and wet; the mean annual values of precipitation, temperature and evapotranspiration are 1715 mm, 14 °C and 807 mm, respectively (Carballeira et al., 1983). The soils
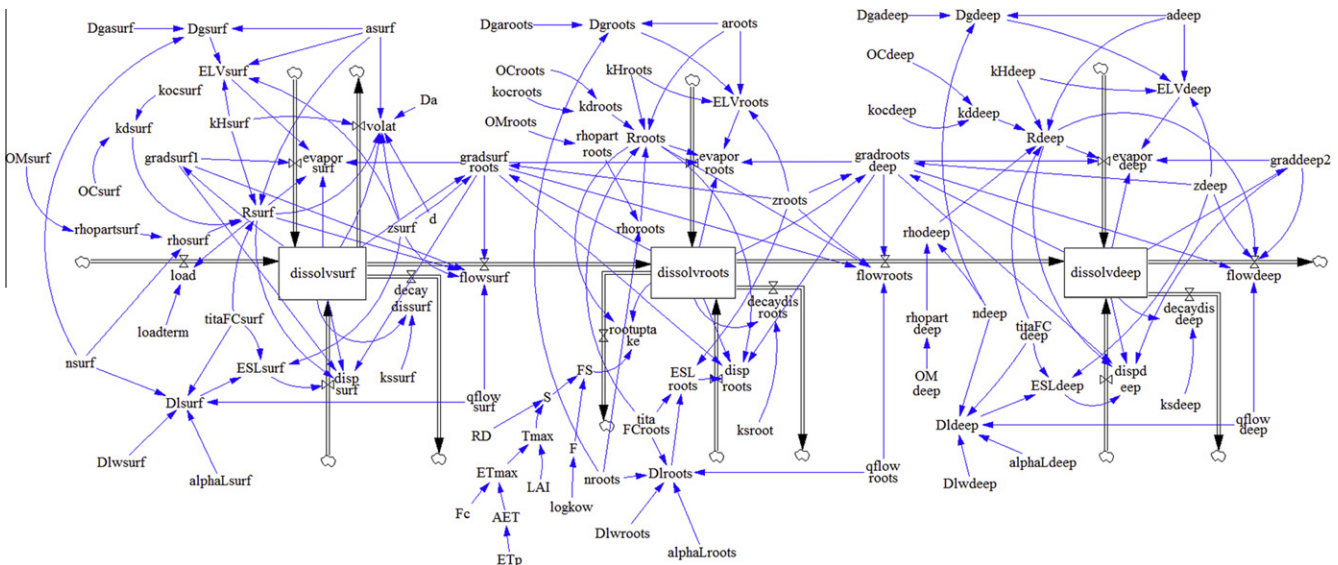

Fig. 2. Configuration of the model by Vensim® software (a specialized System Dynamics programme).

Table 1
Characteristics of the soil profile and initial concentration of lindane in each layer.

Zone	Depth (cm)	Texture[a]	n[b] (cm^3/cm^3)	θ_{FC}[b] (cm^3/cm^3)	% Organic matter	%O.C.	γ-HCH (mg/kg$_{soil}$)
Surface	0–10	Sandy-loam	0.453	0.207	8.76	4.86	2.23
Root	10–75	Sandy-loam	0.453	0.207	7.08	4.11	3.84
Deep	75–95	Sandy-loam	0.453	0.207	0.81	0.47	0.89

[a] Predominant texture in the study area (Calvelo Pereira et al., 2006).
[b] Hydraulic properties provided by Rawls et al. (1992) from texture: n = total porosity of the soil; θ_{FC} = moisture content of the soil at field capacity.

in the plot are Urbic Technosols and/or Technic Regosols (IUSS Working Group WRB, 2007). The site has been the object of previous studies (Calvelo Pereira et al., 2006).

3.2. Model parameters and simplifications: initial conditions for the simulation

3.2.1. Soil and pollutant characteristics

The soil profile was divided into three zones for the simulation: surface (0–10 cm), root (10–75 cm) and deep (75–95 cm). The model assumes that the profile is homogeneous regarding texture, structure and moisture. The profile was contaminated by lindane at concentrations that varied with depth (Table 1).

The values of the basic properties of lindane involved in the transport processes used for the calculations were those reported by Olesen et al. (2001) at 20 °C: vapor-phase diffusion coefficient for the contaminant in free air, $D_g^a = 0.0541$ (cm^2 s^{-1}); dissolved phase diffusion coefficient the contaminant in water, $D_l^w = 5.02 \times 10^6$ (cm^2 s^{-1}); Henry's constant (dimensionless), $K_H = 6.09 \times 10^{-5}$; octanol–water partition coefficient $\text{Log} K_{ow} = 2.81$; organic carbon–soil solution partition coefficient, $K_{oc} = 1081$ (mL g^{-1}).

The degradation constant of the contaminant was calculated by the equation proposed by Sparks (1989):

$$k_s = \frac{Ln2}{\tau_{\frac{1}{2}}} \tag{17}$$

$\tau_{1/2}$ (half-life) is 450 d (FAO, 2000).

The concentrations of lindane in the vapor and dissolved phases were calculated by applying the corresponding partition coefficients (K_H and K_d). Due to the important effect that organic matter has on the sorption of OCPs, the partition coefficient K_d was expressed as a function of the soil organic carbon content (%O.C.) (Chiou, 1989):

$$K_d = K_{OC} \cdot \frac{\%O.C.}{100} \tag{18}$$

The apparent density and the volumetric air content (a) were estimated from the total porosity (n) (Porta et al., 1999):

$$a = n - \theta_{FC} \tag{19}$$

$$n = 1 - \frac{\rho}{\rho_r} \tag{20}$$

The percentage of organic matter was also taken into account to calculate the real density (ρ_r) in each layer (Porta et al., 1999):

$$\rho_r = 2650 - \frac{1450 \cdot \%O.M.}{100} \tag{21}$$

3.2.2. Estimation of drainage in the soil and other hydraulic considerations

Due to the experimental plot was level and small, surface run-off and soil losses through erosion were considered negligible. Thus, the water balance for calculating the net infiltration was:

$$I_{net} = P - ETP - W \tag{22}$$

P is the annual precipitation (mm); ETP is the annual evapotranspiration (mm), and W is the annual amount of water retained by the soil at field capacity (mm), which is calculated by multiplying the volume of the profile considered by the moisture content. The net infiltration represents the mean water flow through the soil, or the mean velocity of water flow, indicated as q in the model.

Another parameter affected by the hydraulic regime of the system is the coefficient of hydrodynamic dispersion, given by the following expression (Bear, 1988):

$$D_l = \left(\frac{\theta^{\frac{7}{3}}}{n^2}\right) \cdot D_l^w + \alpha_L \cdot \frac{|q|}{\theta} \tag{23}$$

This coefficient considers the effects of molecular diffusion and the mechanical dispersion, and includes the parameter of the longitudinal dispersivity of the medium (α_L), which reflects the variation in the migration of the contaminant in the direction of the flow and the consequent expansion of the contamination plume. The longitudinal dispersivity is difficult to determine, and is scale-dependent, and it is therefore usually estimated by the use of empirical expressions (IHOBE, 2006). In the present study, the results of simulations carried out by Sahimi et al. (1986) and the experimental data reported by Haga et al. (1999) were used:

$$\left. \begin{array}{ll} \alpha_L = \alpha_{L_{sat}} \cdot \frac{1}{(Sat)^{2.1}} & Sat > 0.41 \\ \alpha_L = \alpha_{L_{sat}} \cdot [14.6 - 24.3 \cdot (Sat)] & Sat < 0.41 \end{array} \right\} \tag{24}$$

Sat is the real saturation of the medium, calculated as $Sat = \frac{\theta_{FC}}{n}$. The value of the dispersivity at saturation ($\alpha_{L_{sat}}$) was assumed to be 7.8 cm, in accordance with experimental results used in systems of the same order of magnitude as in the present study (Gastó and Grifoll, 2001).

3.2.3. Crop parameters

A barley (*Hordeum vulgare* L.) crop was used for the simulation, as this species is particularly appropriate for phytoremediation in soils contaminated with lindane (Calvelo Pereira et al., 2010).

The assimilation of lindane via uptake of water by the plant roots was calculated as a product of the transpiration stream concentration factor (F) and the water uptake rate (S) (Boesten and van der Linden, 1991).

The expression proposed by Belmans et al. (1983) was used to estimate S:

$$S = \alpha \cdot S_{max} \tag{25}$$

α is a reduction factor (dimensionless), which depends on the moisture content and the hydric potential of the soil (Li et al., 2006), indicating the hydric stress to which the plant is subjected; S_{max} is the maximum rate of water extracted by the roots. Under field capacity, the value of α is considered to be very close to 1, as the amount of water is not limiting (Li et al., 2006).

The maximum rate of water uptake by the roots can be calculated as follows (Nishat et al., 2007):

$$S_{max} = 2 \cdot \frac{T_{max}}{RD}\left(1 - \frac{Z_r}{RD}\right) \quad Z_r < RD \atop S_{max} = \frac{T_{max}}{RD} \qquad\qquad\quad Z_r \geqslant RD \Bigg\} \qquad (26)$$

T_{max} is the potential transpiration rate; RD is the depth of the root front, and Z_r is the depth of the root zone.

If a period longer than the crop growing season is considered, the maximum rooting depth would be reached, and thus $Z_r = RD = 75$cm (simulation invariant). This value is not very different from other rooting depths proposed by Wild et al. (1992) and Canadell et al. (1996) for *H. vulgare* L. T_{max} represents the maximum transpiration value of the crop when water is not limiting, and depends on the maximum evapotranspiration of the crop (ET_{max}) and on the leaf area index (LAI) (Coelho et al., 2003):

$$T_{max} = ET_{max}(1 - e^{-LAI}) \quad LAI \leqslant 3.0 \atop T_{max} = ET_{max} \qquad\qquad LAI > 3.0 \Bigg\} \qquad (27)$$

Different values of LAI have been reported for barley crops, from 0.2 m² m⁻² (Adiku et al., 2006) to 8 m² m⁻² for a crop subjected to phytosanitary treatment (Dammer et al., 2008). FAO (2006) estimated $LAI = 3$ when the crop completely covered the ground, which was initially used in the present simulation.

The evapotranspiration rate (ET_{max}) of a crop depends on the actual evapotranspiration (AET) and can be calculated by taking into account the LAI, applying the correction factor (F_C) proposed by Coelho et al. (2003):

$$ET_{max} = F_C \cdot AET \qquad (28)$$

$$F_C = 1 + 0.074 LAI \quad LAI \leqslant 2.7 \atop F_C = 1.2 \qquad\qquad\quad LAI > 2.7 \Bigg\} \qquad (29)$$

The value of AET at field capacity is consistent with the potential evapotranspiration value (Nishat et al., 2007), calculated from the climatic data (by the Penman method).

Finally, the expression proposed by Briggs et al. (1982), for the assimilation of moderately hydrophobic pesticides by barley, was used to calculate the transpiration stream concentration factor (F):

$$F = 0.784 \cdot e^{[-(\log K_{ow} - 1.78)^2/2.44]} \qquad (30)$$

4. Results of the simulation and discussion

4.1. Contribution of the different flows to the removal of lindane

The simulated concentrations of lindane and the contribution of the considered processes in each of the zones are shown in Fig. 3.

In all three zones, the main route for the disappearance of lindane was the biochemical degradation (*decaydis*); the effect of this decrease was more remarkable during the first years of simulation.

In the surface layer (Fig. 3a) the hydrodynamic dispersion (*dispsurf*) greatly contributes to maintain lindane in the dissolved phase (positive flow) due to the much greater longitudinal expansion of the contamination plume under the moisture conditions considered (FC). The contribution of the hydrodynamic dispersion to the lindane balance was 50% of the initial amount (at the start of the simulation), decreasing rapidly to 20% in favor of degradation, which reached 60% after the first year of the study. These values were maintained for the rest of the study period. The flows by advective transport and infiltration (*flowsurf*) and by volatilization (*volat*), which contribute to the removal of lindane, represent about 10% of the balance each. The decrease due to surface evaporation (*evaporsurf*) accounted for only 0.05% of the exchange of lindane.

In the root zone (Fig. 3b), degradation (*decaydisroots*) was the most important route of removal and represented around 90% of the lindane balance throughout the study period. Infiltration from
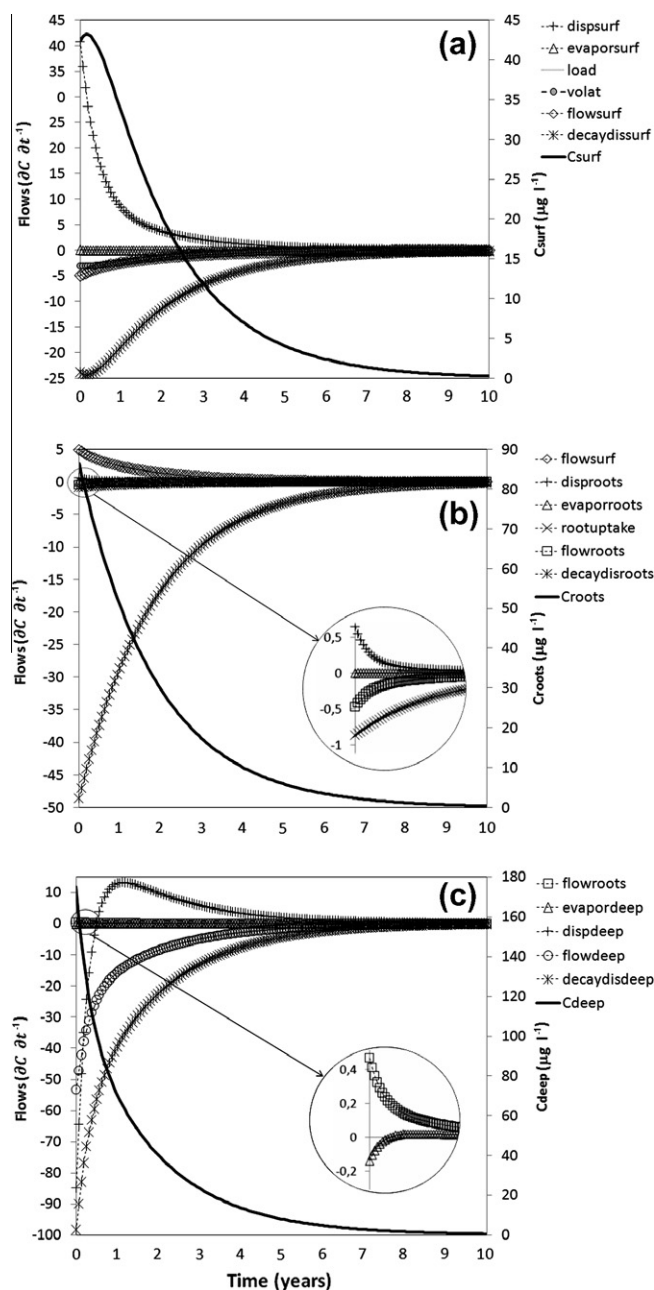

Fig. 3. Changes in the concentration of lindane in the soil solution (C, µg L⁻¹) and relative contribution of the different transport flows ($\delta C/\delta t$) in the three soil zones considered in the model: (a) surface zone (0–10 cm), (b) root zone (10–75 cm), and (c) deep zone (75–95 cm).

the surface zone (*flowsurf*) was around 8%, and the root uptake (*rootuptake*) contributed to the elimination of lindane with a constant 1.6%. The remaining flows accounted for only 0.05% of the lindane in circulation.

In the deep layer (Fig. 3c), the most important phenomenon was still degradation (*decaydisdeep*), accounting for 55% of the balance. The hydrodynamic dispersion in this layer (*dispdeep*) contributed 20% to increase the concentration, and elimination of the dissolved contaminant in the deep infiltration flow (*flowdeep*) accounted for another 20%. The latter output flow will contribute to the gradual contamination of water below the soil profile, contributing an amount of lindane that will vary from values higher than 130 g per year, at the beginning of the simulation, to 0.25 g per year after 10 years.
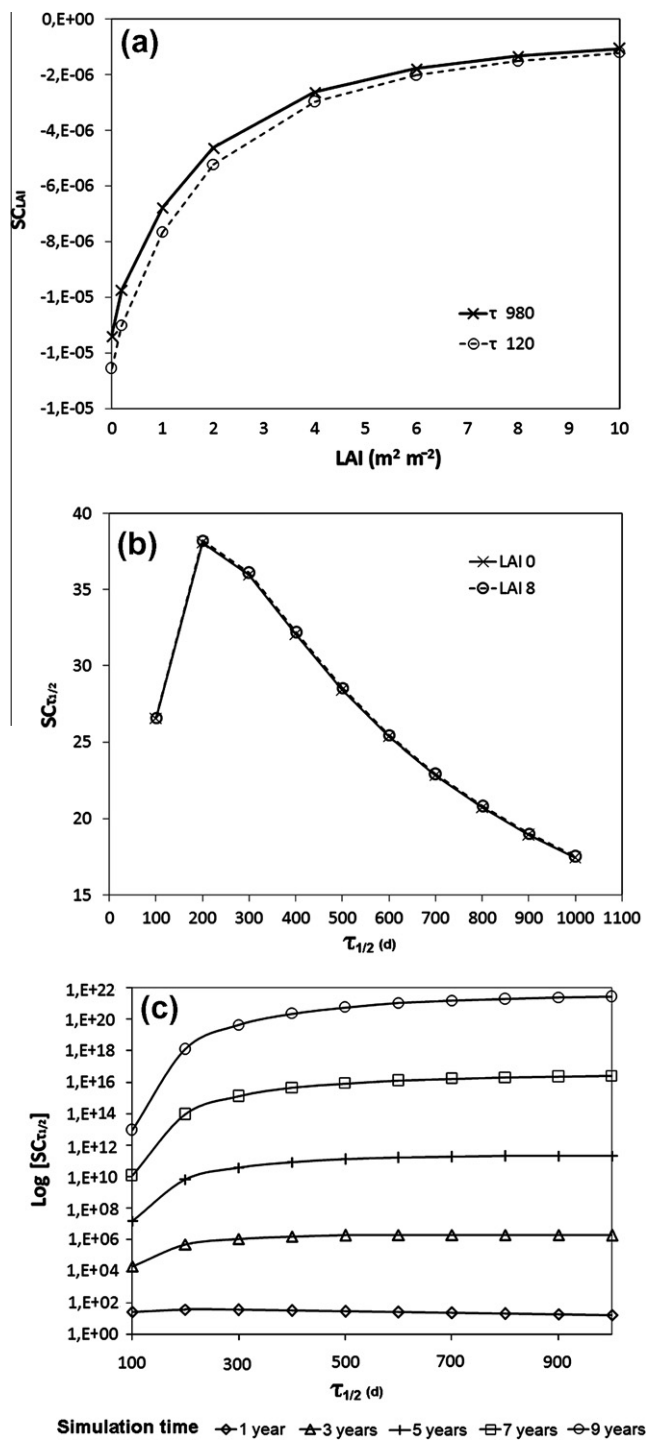
Fig. 4. (a) Sensitivity of the model to the leaf area index, for two extreme values of the half-life of lindane; (b) sensitivity of the model to the half-life of lindane, for two extreme values of leaf index area; (c) sensitivity of the model to variations in the half-life of lindane, for different simulation periods.

4.2. Sensitivity analysis

One of the benefits of Vensim® is the possibility of assessing the change in the model response by varying the value of several parameter, which facilitates sensitivity analysis. In this study, the sensitivity of the model regarding *LAI* and $\tau_{1/2}$ was tested within the first year of simulation in root zone.

The sensitivity coefficient was calculated as (Behrendt et al., 1995; Ao et al., 2009):

$$SC_i = \frac{\Delta Y_i/Y_i}{\Delta X_i/X_i} \tag{31}$$

SC_i represents the ratio between the relative variation in the system response (Y_i) and the relative variation in a parameter of the model (X_i). Values of SC_i higher than zero indicate an increase in the concentration of lindane in the dissolved phase of the root zone, while negative values indicate a decrease.

After 1 year of simulation, the results indicated that the model was much more sensitive to variations in the half-life of lindane than to variations in *LAI* (Fig. 4) ($\overline{SC}_{LAI} = -5.1 \times 10^{-6} \pm 4.1 \times 10^{-6}$; $\overline{SC}_{\tau_{1/2}} = 26.7 \pm 7$).

The negative values obtained for SC_{LAI} (Fig. 4.a) indicate that with increasing values of *LAI*, the concentration of lindane predicted by the model decreases, although the variation is minimal, and only more pronounced for values of *LAI* < 3. This indicates that even if the crop reaches a higher level of foliar vigor, this will not significantly increase the removal of contaminant, and scarce differences were observed on varying the value of the half-life of the compound.

The high values of $SC_{\tau_{1/2}}$ obtained (Fig. 4b) indicate the high sensitivity of the model to the half-life of lindane, with a maximum of 200 d for $\tau_{1/2}$. So that increases in this parameter would lead to higher concentrations of the compound in the soil. This $SC_{\tau_{1/2}}$ would not be affected by extreme values of *LAI*. Other authors have also reported the great dependence of these models to the degradation term (Behrendt et al., 1995) and also that the sensitivity may vary over time (Ao et al., 2009). The $SC_{\tau_{1/2}}$ was therefore analyzed for the whole simulation period (Fig. 4c), and the sensitivity coefficients obtained increased with the time of simulation, and were different between each other by five orders of magnitude ($\overline{SC}_{\tau_{1/2}} = [2.7 \times 10^1]_{t=1\,year}$; $[1.5 \times 10^6]_{t=3\,years}$; $[1.2 10^{11}]_{t=5\,years}$; $[1.1 10^{16}]_{t=7\,years}$; $[1.0 10^{21}]_{t=9\,years}$). This indicates a high degree of uncertainty in the prediction of the behavior of the system, as there is no general consensus regarding the value of the half-life of lindane in soil, which depends on several factors (type of soil, climatic condition, temperature, moisture, biological activity, soil use, etc.). Values ranging from a few days to three years have been reported (UNEP, 2006).

5. Conclusions

System Dynamics allowed to assess trends in the behavior of a soil–plant system contaminated with lindane and also to evaluate which parameters or processes are more important for its dissipation. This facilitates more appropriate decision to future assays to remediation of contaminated soils.

The high accessibility and interactivity of Vensim® facilitated the modeling of a polluted soil. It permitted a good understanding of the behavior of the system through visualization of all of the variables and feedback relationships, which is sometimes not possible with other types of simulation tools, while allowing for sensitivity analysis.

Decreasing of lindane in soil is mainly due to biochemical degradation, although infiltration also contributes significantly to the removal of pollutant. Hydrodynamic dispersion contributes to maintain lindane in the soil, particularly in the surface and deep zones. Uptake of lindane via the roots of vegetation does not contribute greatly to its removal, due to its low solubility and strong sorption by soil organic matter.

The half-life proved to be a key parameter. We must research different ways of reducing its value and thus enhance the removal of the pollutant from the soil, such as biological processes that would stimulate the biodegradation of the pollutant. Implementation of expressions to simulate these processes should be included

in the current model to determine the extent of their contribution to removal.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.chemosphere.2012.10.082.

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