



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

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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.

ARTICLE INFO

Article history:

Received 23 February 2012

Received in revised form 29 September 2012

Accepted 17 October 2012

Available online 22 November 2012

Keywords:

Environmental modelling

Vensim

Persistent pesticides

Contaminated soils

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.

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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 (Kozioł 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

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(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.

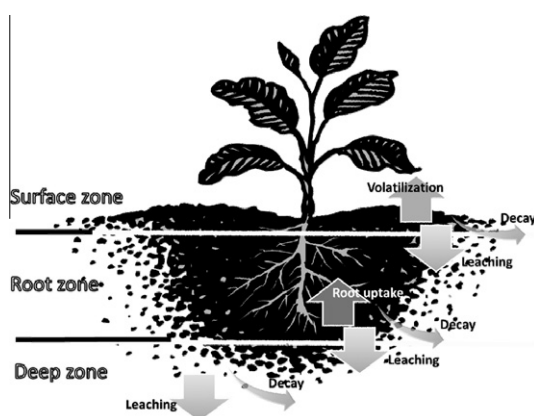


Fig. 1. Conceptual model of pollutant fate in soil.

The mathematical expression of the model is as follows:

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

C = concentration of contaminant in the soil solution [ML^{-3}]; θ = volumetric water content of the soil [$L^3 L^{-3}$]; a = volumetric air content of the soil [$L^3 L^{-3}$]; ρ = apparent density of the soil [ML^{-3}]; K_d = distribution coefficient [$L^3 M^{-1}$]; K_H = Henry's constant (dimensionless); D_g = coefficient of diffusion of the contaminant in the vapor phase [$L^2 T^{-1}$]; D_l = coefficient of diffusion of the contaminant in the dissolved phase [$L^2 T^{-1}$]; D_g^a = coefficient of diffusion of the vapor phase of the contaminant in the open air [$L^2 T^{-1}$]; 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 [$L^3 L^{-3} T^{-1}$]; 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:

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

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

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

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

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

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®:

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