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Exploring improved pesticide management in sub-tropical environments with GIS-supported fate modeling

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Abstract

The sensitivity analysis of pesticide models to input parameters related to crop management practices supplies working hypotheses to improve pesticide uses and environmental quality. Parameters of pesticide models that are influential to model output vary depending on regional environmental conditions, and their probability distribution functions must be identified on a case-oriented basis. While the performance of pesticide models has been extensively tested in temperate regions, comparative studies in subtropical areas are relatively scarce. In this study, we coupled results of landscape analyses supported with a geographical information system (GIS), field data and information about management scenarios of citrus crops in Misiones (Argentina) to inspect the behavior of a field-scale pesticide model (GLEAMSv3.0). Probability distribution functions of model parameters relevant to hydrology, geo-forms and crop distribution were derived from satellite imagery (SAC-C, SRTM), while crop characteristics, information on soils and pesticides were obtained from field data. Spatial descriptors were used to generate sensitivity scenarios to explore the potential effect of management practices on the fate of the pesticides chlorpyrifos, mancozeb, mercaptothion, copper hydroxide, carbendazem, glyphosate and 2-4-D used in citrus crops. Our results indicate that management practices to change the roughness-contouring of the soil, maintaining a high vegetation cover below the citrus crops, and devising pesticide spraying techniques that would

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efficiently increase the contact with the crop leaves would be expected to significantly reduce pesticide losses. Plant spacing, improving soil textural conditions through soil-correction practices and selecting adequate soil conditions for installing new crops are also potentially effective techniques to the same goal. Glyphosate losses are almost insensitive to management manipulation, which is a favorable trait in cases where management alternatives are constrained by practical or economic considerations. We present comparisons of the sensitivity of the pesticide model in these scenarios in relation to previously reported results with the same model in other cases, and formulate proposals on a normalized format to report sensitivity results to facilitate comparisons among models and cases.

Keywords: Pesticide management; Pesticide models; Sensitivity analysis; GLEAMSv3.0; Subtropical crops; GIS modeling

1. Introduction

Pesticide models like GLEAMSv3.0 (Knisel and Davis, 2000) and others with similar rationale were developed for use as research and management tools for the estimation of pollutant losses from agricultural systems. A key aspect in these applications is the evaluation of the sensitivity of the model output to input parameters. This is usually performed in a context of model validation and error prediction (Wolt et al., 2002). In the case of models that have already been extensively tested in these respects, the analysis of the model response to variations of the input parameters is useful to formulate testable hypotheses for experimentation on improved management techniques, site and pesticide selections and the adequate timing of applications and monitoring guidelines. In the case of GLEAMS, the sensitivity of a preceding version (GLEAMS, v2.1) with similar structure has been tested to explore model uncertainty (Knisel, 1993;Wedwick et al., 2001) and behavior in landscape and management related contexts (Searing et al., 1995;de Paz and Ramos, 2001).

Subtropical environments are characterized by climate regimes with intense and frequent precipitation events and high ambient temperatures. These influence fast growth rates of both crop plants and their pests, low soil organic matter contents and potentially high rates of soil erosion and sediment transport. All these traits are highly influential in the fate of agricultural pesticides, although relatively few studies have evaluated the sensitivity of pesticide fate models in subtropical regions. Pesticide management in subtropical areas could benefit from sensitivity results that would indicate which of the model parameters related to management practices are most influential in pesticide environmental losses.

Sensitivity analyses involve the selection of a set of model input parameters (the so-called sensitivity shell) and the inspection of the variations of some relevant model output class (the sensitivity response) to forced fluctuations of the parameters in the shell. Current available and well tested pesticide models incorporate key parameters related to soil, climate and management conditions as well as pesticide thermodynamic data (Yulianti et al., 1999). Since complex interrelations exist among many of the parameters, the identification of the model sensitivity is not absolute, but depends on the parameter list within the sensitivity shell, their ranges of variation and statistical distributions. As a result, sensitivity studies on a same model can identify dissimilar lists of influential parameters depending on the modeler's objective and the modeled scenario (Leonard et al., 1987;Leonard et al., 1992;Knisel, 1993; Zacharias and Heatwole, 1994;Ma et al., 2000).

Modeling techniques based on Monte Carlo (MC) sampling can be used to investigate model sensitivity (relations between model input and output) and model uncertainty (variability of results depending on uncertain input parameters) (Carbone et al., 2002; Warren-Hicks et al., 2002). A key aspect in MC-sensitivity analysis is the selection of adequate probability distribution functions (PDFs) of the tested parameters. PDFs of input parameters are necessarily conditional to each other, since most environmental variables cannot be considered as independent in a statistical sense. Dubus and Janssen (2003) have recently summarized recommendations for an adequate structure of MC-sensitivity analysis. Although in some cases the PDFs are estimated through expert judgment, they should represent, to the degree possible, the actual site-specific patterns of variation. They should also span the range of possible values of the parameters for the objective of the sensitivity analysis and the form of the selected sampling distribution should be consistent between sites for a specific parameter. Last, the form of the distribution should reflect the magnitude, range, and interpretation of the parameters. Many of the input parameters have restricted ranges and care should be exerted in precluding the choice of non-feasible parameter values or ranges, since unreal variation ranges can generate artifact sensitivities.

This study uses field information on usual management practices in citrus crops in the sub-tropical region of Misiones (Argentina), spatial descriptors of landscape characteristics (soil quality, geomorphology, hydrology), crop distribution data and sensitivity analyses of a pesticide fate model to construct working guidelines for improved pesticide management in this environment. Satellite imagery and complementary sources of landscape information (charts and geo-referenced land surveys) are used to identify the locations of the crop. A digital elevation model (DEM) is used to characterize the landscape as needed for the analysis of surface water flows, a major driving force of pesticide fate. Observations on the predominant management practices related to the condition of the upper soil layers, its vegetative cover, the spacing of crop trees and the timing of pesticide applications in relation to meteorological events are used to define pertinent model parameters. Specifically, we address the question of what management practices have the potential to minimize pesticide losses in citrus crops in Misiones.

2. Materials and methods

Fig. 1 presents a schematic overview of the procedures followed in this study. Field surveys supplied information on the ground truth position of sample citrus crops and soil characteristics (Sections 2.1, 2.3). Remotely sensed imagery was used to generate topographic images through digital elevation modeling (Section 2.2). and mapping all citrus crops over the Misiones region (Section 2.3). PDFs of model

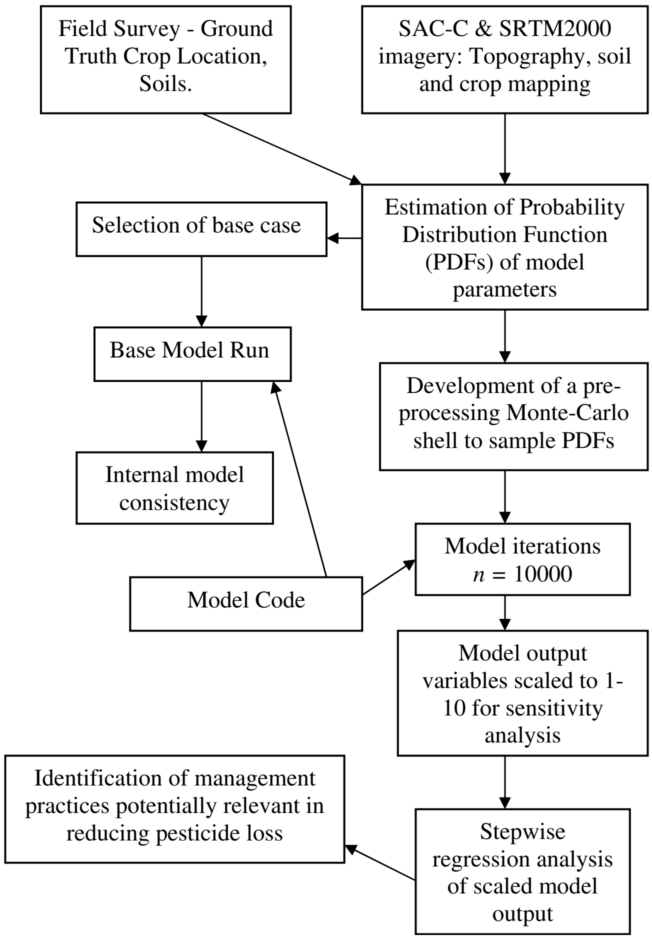


Fig. 1. Schematic summary of the procedure used in this study.

parameters related to soil and topography were estimated by the joint use of both (Section 2.4), and a model run corresponding to a modal case was performed to test for internal model consistency (Sections 2.5, 3.1). PDFs were built into a model pre-processing computer routine (Section 2.7), and model output variables were scaled and inspected for sensitivity through stepwise regression analysis (Section 2.7). Potentially relevant management practices to reduce pesticide losses were then identified (Section 3.2).

2.1. Regional field data

The region inspected in this study is the Province of Misiones in Argentina, located within the 25°28′S–28°10′S and 53°38′W–56°03′W at the north-eastern border of Argentina. Gentle slopes and small hills resulting from past intense erosion characterize its relief. Average altitudes are from 800 m at the northeast to 100 m in the south. Sloping plains crossed by wide fluvial valleys occupy most of the area (Fig. 2). In recent years, citrus crops (tangerine, lemon, orange) have attracted the interest of farmers and demand intensive use of pesticides to control their many pests (SAGPyA, 2000).

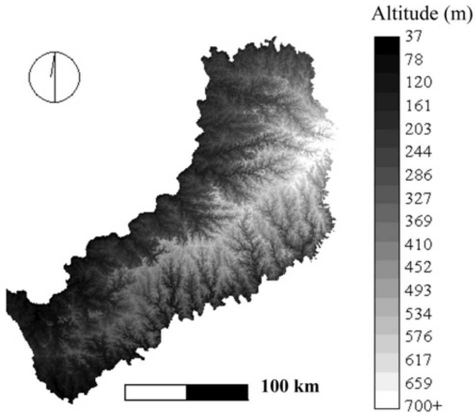
The climate is subtropical warm with abundant precipitation (150–200 cm/year) and no marked dry season. The average air temperature is 20–21 °C, with 11 °C annual amplitude. This combination of abundant precipitation and high temperatures favors vigorous growth of many plant species as well as of their pests. Also, a fast environmental transport of water-soluble substances and metabolites can be expected as well as their movement with water eroded sediments and top soils. The high frequency of precipitation events also limits many farm tasks including pesticide spraying. Daily precipitation records (1973–2002) for this study were obtained from the Cerro Azul Agricultural Experimental Station (27°39′S, 55°26′W) of the National Institute of Agricultural Technology, Argentina.

2.2. Topography, shapes and slopes

A digital elevation model (DEM) of Misiones (Fig. 3a) with resolutions 90 m, 90 m, 1 m (x, y, z, respectively) generated by the SRTM shuttle radar satellite was

Fig. 2. Situation of subtropical Misiones Province (Argentina) in the South-American continent.

a



b

#, Diagram	Topo-shape name	Drainage area *DAOVR* (ha)	Max. Slope length XOV, XSOIL (m)	#, Diagram	Topo-shape name	Drainage area *DAOVR* (ha)	Max. Slope length XOV, XSOIL (m)
1	Peak	27.54	252	7	Hillside - Convex	12.24	252
2	Ridge	21.42	252	8	Hillside-Saddle	12.24	175
3	Saddle	9.18	175	9	Hillside-Slope	12.24	252
4	Flat	3.06	82.5	10	Hillside-Concave	3.06	82.5
5	Ravine	3.06	82.5	11	Hillside-Inflection	18.06	252
6	Pit	3.06	82.5				

Relative altitude: High Medium Low

Fig. 3. (a) Digital elevation model (DEM) of Misiones Province. (b) Water flow routing types for use with GLEAMSv3.0 defined on 3×3 cell kernels of the DEM at a spatial resolution x, y: 175 m, 175 m (3.06 ha). Parameter values are calculated with respect to the central pixel of each kernel. The drainage area is defined as the area of the central cell + the area of all cells potentially reached by a water flow starting on it, if any. Local soil slopes and toposhape images (not shown) were derived from a.

used to infer local slopes (Monmonier, 1982). One out of eleven basic topographic shapes (Fig. 3b) was then assigned to the central pixel of every 3×3 kernel of the image. Slope and topo-shape images (not shown) were then constructed (Eastman, 2001).

In what follows, italicized acronyms correspond to the names of variables in GLEAMS code. A relative overland condition was assigned to the central element of each kernel and local drainage areas (*DAOVR*) and absolute and relative slope-lengths (*XOV, XSOIL*) were calculated considering the number of pixels in the kernel that could receive runoff water from the central element and the maximum length of feasible flow paths.

2.3. Soils and citrus crop mapping

Most soil types in Misiones derive from basalt rocks, with minor representation of other soil groups originated from sandy sedimentary deposits and fluvial sediments. A soil subgroup map (Fig. 4a) and corresponding data (Table 1) were obtained from the available local soil survey (Ligier et al., 1990).

Most citrus crops occupy nearly flat or gently sloping areas in the numerous valleys crossing the territory, usually on Rhodic Kandiudulth, Kanhapludalf, Typic

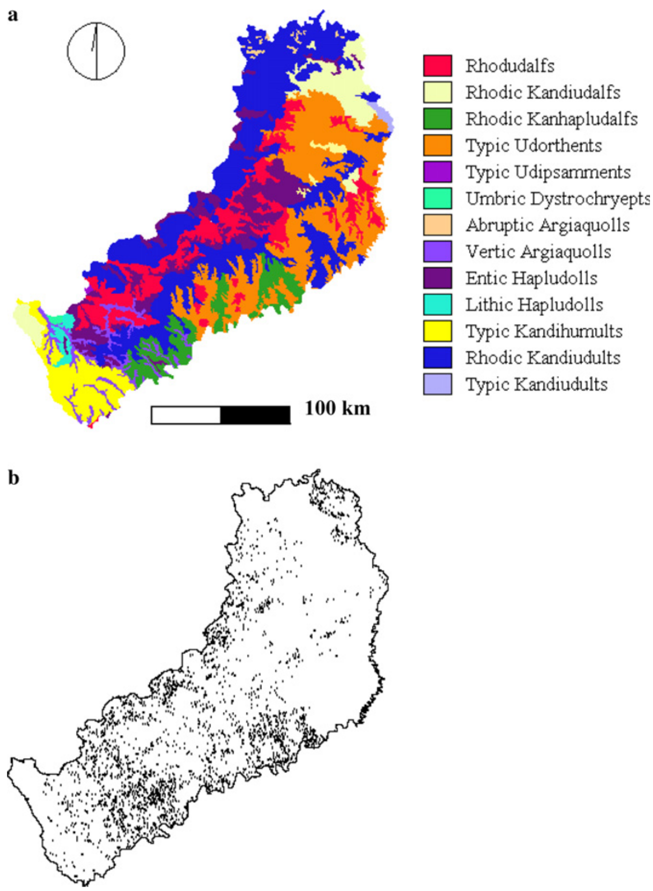


Fig. 4. Some basic layers of the GIS (geographical information system) procedure used to estimate the probability distribution functions of soil parameters corresponding to areas occupied by citrus crops in Misiones. (a) Soil subgroup distribution. (b) Locations with citrus crops (black dots).

Table 1
Modal characteristics of main soil subgroups where citrus crops are raised in Misiones used to run the GLEAMS model in this study

	Rhodic Kandiudults	Rhodic Kanhapludalfs	Typic Udorthents	Rhodudalfs	Entic Hapludolls	Vertic Argiaquolls	Typic Kandihumults	Rhodic Kandiudalfs
Texture of the upper horizon	Clay	Clay	Loam-clay loam	Clay	Loam-clay loam	Clay loam-clay	Clay	Clay
Hydrologic group	D	D	C	D	C	D	D	D
H1 Depth (cm),	6	10	10	6	20	15	10	10
H1 clay (%),	50	50	35	50	20	35	50	50
H1 silt (%)	30	30	30	30	35	30	30	30
H1 Organic matter (%)	4	3	3	4	5	4	6	3
H2 Depth (cm)	12	20	30	12	40	30	23	20
H2 clay (%)	50	50	35	50	20	35	50	50
H2 silt (%)	30	30	30	30	35	30	30	30
H2 Organic matter (%)	3	2	3	3	4	3	4	2
H3 Depth (cm)	100	60	75	100	100	45	100	60
H3 clay (%)	50	50	15	50	5	40	50	50
H3 silt (%)	30	30	25	30	5	35	30	30
H3 Organic matter (%)	2	1	1	2	2	2	3	1
H4 Depth (cm)	>150	>100	350	>150	–	80	>100	150
H4 clay (%)	50	50	15	50	–	45	50	50
H4 silt (%)	30	30	25	30	–	35	30	30
H4 Organic matter (%)	1	1	1	1	–	2	2	1

Udorthent, Entic Rhodudalf and Entic-Lithic Hapludoll soils. They are sparsely distributed among other land uses and crops and vary in terms of their age and development, the distance at which the trees are planted (3–7 m), the co-cultivation with other crops of lower height (e.g., tobacco) or the extent to which the spontaneous growth of native or planted herbaceous undercover is controlled.

In order to map citrus at a regional scale, we obtained two raw SAC-C images (dated 13 October 2001, 2 February 2002) covering the whole territory of Misiones Province. After adequate pre-processing (geo-referencing, radiometric calibration as in García and Chuvieco, 2003), we identified the location of 80 citrus crops (GPS, Garmin 12, Garmin International Inc., Olathe, Kansas, US) in the main production areas in Misiones (San Ignacio, San Martín, Monte Carlo, El Dorado, L. Alem) within 54°36′ to 55°27′W and 27°20′ to 26°14′S (about 1 million ha). Occurrences of other land cover types (tea, yerba (*Ilex sp.*), planted forests, natural forests, urban and suburban areas) were also recorded at additional 200 observation points selected as adequate during the field search. A training image for the identification of citrus crops was created based on the positions of a random subset of 40 of the visited crops and a signature for this crop was developed with the values of the training sites in a set of images calculated from the bands of both SAC-C images as in Pinti and Verstraete (1992). A supervised classification of the images aimed to generate estimates of belief and plausiblity (Eastman, 2001) scores of citrus and non-citrus areas was performed through Bayesian inference (Gordon and Shortliffe, 1985) according to a Dempster-Shafer algorithm (Duda et al., 2001). The image of citrus belief scores was further reclassified to show just the 3.135 pixels (corresponding to 9600 ha, the reported area occupied by citrus crops, SAGPyA, 2000) and overlayed with a co-registered point vector file containing the 40 citrus locations that had not been used to construct the signature for the classification process. The average error incurred in positioning this latter set of citrus crops was ±55.5 m ($p \leqslant 0.05$) (Fig. 4b). The result of this analysis were used to cross-tabulate relief and soil properties at places where citrus are grown, for the sake of the sensitivity analysis of parameters related to crop management practices.

2.4. Probability distribution functions

The image of soil subgroups (Fig. 4a) was digitized by assigning a consecutive number (1–14) to the classes in the order in which they appear in the figure legend, and was cross-tabulated with the citrus-location image (Fig. 4b) to identify the frequencies of major soil subgroups on which citrus are grown.

Analogously, the frequencies of occurrence of topographic shape classes in areas occupied by citrus crops were calculated by further cross-tabulation with the image of the topo-shapes. The frequencies of various slope classes corresponding to each topo-shape were obtained through a similar cross-tabulation. Explicit (exponential, normal) conditional probability distribution functions (PDFs) were fitted to the observed frequency distributions (PEAKFIT Software, SPSS Inc., Chicago, US). The cross-tabulation procedure generates only those combinations of soils,

Table 2
Functional forms of the probability distribution functions fitted to field data and further used in pre-processing of the MC-sensitivity shell for GLEAMS stochastic runs

Analytical form	a_0	t-value	a_1	t-value	a_2	t-value	DF	r^2
a. $y = a_0\exp(-x/a_1)$	0.603	65.525	2.017	9.513	–	–	1, 12	0.956
b. $y = a_0\exp(0.5((x - a_1)/a_2)^2)$	0.391	13.713	8.410	89.940	1.277	13.481	2, 39	0.731
c. 2. $y = a_0\exp(0.5((x - a_1)/a_2)^2)$	0.148	16.280	2.994	8.055	3.127	7.809	2, 6	0.913
5. $y = a_0\exp(0.5((x - a_1)/a_2)^2)$	0.160	24.145	2.338	6.658	3.190	9.774	2, 6	0.964
7. $y = a_0\exp(0.5((x - a_1)/a_2)^2)$	0.122	14.937	4.842	23.571	2.626	10.774	2, 6	0.882
8. $y = a_0\exp(0.5((x - a_1)/a_2)^2)$	0.125	14.512	4.713	21.312	2.719	10.117	2, 6	0.866
10. $y = a_0\exp(0.5((x - a_1)/a_2)^2)$	0.128	11.209	4.833	16.217	2.823	7.57	2, 6	0.776
11. $y = a_0\exp(0.5((x - a_1)/a_2)^2)$	0.153	7.326	4.381	10.742	2.519	5.331	2, 6	0.646

't' values of the fitted parameters significant at $p \leqslant 0.05$. a. Probability (y) distribution function of soil subgroups (x) in citrus crops. b. Same of toposhapes (x) in soil subgroups under citrus crops c. Same of slope classes (x) in soil toposhapes in soil subgroups under citrus crops in toposhapes 2, 5, 7, 8, 10 and 11.

toposhapes and slopes that actually occur in existing citrus crops. Table 2 summarizes the analytical form of the PDFs used in this study.

2.5. Model run of modal case

We used the public version of GLEAMSv3.0 code, related parameter-file editors (climate, hydrology, erosion, pesticides) and pesticide thermodynamic data-base to perform simulations of pesticide fate in citrus crops in Misiones. Additionally, we incorporated $Cu(OH)_2$ to the base with thermodynamic data as in Perry and Green (1973) and Buchter (1989). GLEAMS is physically-based except for the use of curve-number based hydrology, and is designed to be applied at the field-scale, although a field in terms of the model conceptualization is not strictly the area planted with a crop but rather that corresponding to the whole drainage system associated to it. The assignation of parameter values is deterministic, and testing parameter sensitivity with the available code requires repeated independent model runs.

Based on a preliminary inspection of the frequency distribution of soil subgroups, soil topographic shapes within soil subgroups, and soil slope classes within topographic shapes in citrus crops, a modal case (Table 3) corresponding to the most frequent class of all distributions in Table 3 was selected to perform a base model run. Pesticide application rates to citrus crops as based on agronomic recommendations by the Misiones Provincial Ministry of Agriculture were adopted for model input (Table 4). Time-windows to apply pesticides were defined by setting 8 target days/year evenly spaced along the growing season, and postponing each of them at one-day iteration steps depending on the occurrence of storms heavier than 0.5 cm of rain up until a non stormy day occurrence, in a way similar to what farmers in Misiones usually do.

2.6. Pre-processing MC-simulations

The analyses of the sensitivity of GLEAMSv3.0 to management-related parameters were performed by running the model with a set of randomly sampled input

Table 3
Selected parameter values used to generate a base GLEAMSv3.0 model run. Climate variables correspond to the period 1973–1975 (Cerro Azul Agro-Meteorological Station)

Parameter	Value	Units	Definition
FLGGEN	0	cm/day	Evapotranspiration (Priestley-Taylor algorithm)
FOREST	3	–	Forest-perennial crop type of application
RC	0.05	cm/h	Effective saturated conductivity of soil horizon immediately below the root zone.[a]
CONA	3.0	–	Soil Evaporation parameter.[a]
CN2	89	–	SCS Curve number.[a]
CHS	0.03	m/m	Hydraulic slope of the field as inferred from conditional frequency distribution under citrus crops.[b]
WLW	0.25	–	Ratio of field length to field width as inferred from toposhape frequency distribution.[b]
NSOHS	4	–	Number of soil horizon layers (Depths (cm) 0–6, 6–12, 12–100, 100–150).[c]
POR	0.39	cm^3/cm^3	Porosity of soil profile.[a]
FC	0.38	cm/cm	Field capacity of the soil profile.[a]
BR15	0.28	cm/cm	Wilting point of the soil profile.[a]
SATK	0.05	cm/h	Effective saturated conductivity of the soil profile.[a]
OM	4-1	%	Organic matter content of soil horizon layers.[c]
CLAY, SILT	50–30	%	Clay and silt content in the soil profile.[c]
TEMPX, TEMPN	31.5–10.9	°C	Maximum-Minimum monthly average air temperature.[d]
RAD	2100–830	mJ/cm^2	Mean monthly global radiation.[e]
WIND	144–103	km/day	Mean monthly wind movement.[e]
DEWPT	21.0–11.0	°C	Mean monthly dew point air temperature.[e]
CCRD	1.5	m	Citrus crop estimated rooting depth
CCRPHTX	2	m	Citrus crop height
CFACT	0.01	–	Ratio of soil loss relative to that under continuous fallow.[a]
PFACT	0.5	–	Contouring factor.[a]
NFACT	0.045	–	Manning's parameter for overland flow.[a]
LAI	4	m^2/m^2	Leaf area index.[f]
FOLFRC	0.7		Fraction of pesticide application rate onto leaves vs. onto soils

[a] Model documentation, inferred for Rhodic Kandiudults.
[b] Table 1, this study.
[c] Table 2, this study.
[d] Average period 1973–2002. Cerro Azul Agro-Meteorological Station.
[e] Average period 2000–2002. Cerro Azul Agro-Meteorological Station.
[f] Cohen and Fuchs (1987).

parameters within the estimated PDFs and ranges as described above. This required re-writing some parts of the input code in order to define default parameter file names to allow automation of GLEAMSv3.0 runs and coupling to a pre-processing MC-shell subroutine developed for this purpose. The subset of input parameters to be included in the MC-shell (Table 5) was selected based on several criteria. Some parameters were selected because they would refer to elements or mechanisms that could to some extent be under the control of the farmers. Examples of these are

Table 4
Main pesticide types and recommended rates of application for use in citrus crops in Misiones province

Recommended for treatment of	# treatments per year	Product[a]	Appl. rate (kg ha^{-1})	Comments	Average annual rate[b] (kg ha^{-1})
Fungii	7–8	$CuOH_2$ (77%)	15.5 × 7	Average	83.5
Fruit fly	5–7	Mercaptothion, (100%)	3.82 × 5	Average after 4th year	19.1
Insects	8	Chlorpyrifos, (48%)	1 × 8	After 4th year	3.84
Fungii	8	Mancozeb, (80%)	15 × 8	Every year	96
	8	Carbendazim, (75%)	4 × 8	Average after 4th year	24
Weeds	8	Glyphosate, (48%)	3.4 × 8	Every year	13.1
	8	2-4-D, (100%)	3.4 × 8	After 3rd year	27.2

[a] Expert recommendations are usually formulated in terms of commercial formulations for ease of interpretation by farmers. The applied doses can vary considerably from case to case, depending on the equipment used, personal criteria and other factors. Accordingly, the numbers here presented should be considered as educated guesses of the actual amounts used. In all cases, 700 L/ha application volumes are assumed.

[b] As active product. Average over 30 years.

Table 5
Ranges and distributions of variables used to generate MC-input to GLEAMSv3.0

Input parameter, acronym	Meaning	Units	Range	PDF
APPL. RATE	Applied pesticide	kg/ha, 3-year period	See Table 4	Linearly related to LAI + random uniform around 1/2 range
BOTHOR1	Depth of upper layer of soil profile	cm	12.0–40.0	Exponential
BR151	Water content of upper soil layer at wilting point	cm/cm	0.29–0.29	Uniform
CHS	Hydraulic slope of the field	m/m	0.01–0.09	Normal within topo-shape range
CLAY1	Percentage of clay in upper soil layer	%	20–50	Exponential
CN2	Soil curve #		80–89	Uniform within range of texture class
CRPHTX	Crop height	m	1.5–3.5	Uniform within range
FC1	Water content of upper soil layer at field capacity	cm/cm	0.39–0.39	Uniform
FOLFRC	Fraction of the applied pesticide effectively reaching the foliage of target plants (either citrus or undergrown weeds)		0.15–0.94	Linearly related to LAI + random uniform around 1/2 range
KSOIL	Soil erodibility factor for slope segment		0.245–0.275	Exponential
LAI	Leaf area index (m/m)	m/m	1–7	Random uniform within range
NFACT	Manning's factor for overland flow path		0.015–0.40	Random uniform within range
OM1	Percentage of organic matter in upper soil layer	%	2–4	Exponential
POR1	Porosity of upper soil layer	cm^3/ cm^3	0.45–0.45	Uniform
RC	Effective saturated conductivity of the soil profile	cm/hour	0.07–0.25	Exponential
SATK1	Saturated water conductivity of upper soil layer	cm/hour	0.05–0.20	Exponential
SILT1	Percentage of clay in upper soil layer		30–35	Exponential
SOILLOSS	CFACT Soil loss ratio for overland flow segment		0.01–1.0	Uniform within range
SSCLY	Clay specific surface	m^2/g	10–999	Uniform within range
WLW	Length–width ratio of drainage sub-basin		0.22–0.52	Log-normal

the fraction of pesticide effectively applied to the plant canopies (*FLFRC*), the state of soil cover and resulting *CN2* soil curve number, and the leaf area index of the crop (*LAI*) resulting from tree spacing. A second group of selected parameters referred to relevant soil characteristics, because farmers could orient the selection of suitable new sites for citrus crops or selectively recycle those old crops presently installed in less suitable areas. Examples of these latter are terrain slopes/relative slope-lengths (*CHS, WLW*) and depth-quality of the upper soil layer (*BOTHR1, OM1, CLAY1*). A third group of selected parameters for MC-testing was chosen based on the scarcity of available information on their values, mostly because they are not incorporated in routine soil surveys. Examples of these are the specific surface of soil clays (*SSCLY*) or the effective saturated conductivity of the whole soil profile (*RC*). In what follows, specific comments relative to the model input parameter files are detailed.

At each iteration, a sample series of three consecutive years of daily rainfall and maximum–minimum temperature data was randomly drawn from the climate data series (Cerro Azul Agro-Meteorology Station site, 1973–2002) in order to account for interannual climate variability. A soil subgroup was then selected at each model iteration by drawing a random case from the corresponding conditional PDF, as well as a uniform random soil curve number (*CN2*) within the range described for the selected soil subgroup-texture class. A topographic shape was then drawn from the respective PDF as well as feasible slope value (*CHS*) from the topo-shape specific PDF. A drainage area (*DAOVR*) and its length–width ratio (*WLW*) were then updated according to Table 1 as well as the soil profile saturated conductivity (*RC*), depth of the soil horizons (*BOTHOR*), clay–silt–organic matter content (*CLAY, SILT, OM*), porosity (*POR*), saturated and wilting point water contents (*FC, BR15*) as estimated from soil pedotransfer fuctions (Saxton et al., 1986). Leaf area indexes (*LAI*) were drawn from a uniform distribution within the range 1.5–7, as estimated from field observation and reported values for citrus crops (Cohen and Fuchs, 1987).

The specific surface of clay in the soil profile (*SSCLY*), Manning's overland (*NFACT*) and soil loss-factors (*CFACT*) were drawn from uniform distributions within ranges estimated with pedotransfer functions (Saxton et al., 1986) and suggested in the model documentation or characteristic for the soil hydrologic group or corresponding texture class. The operation of the erosion routine of GLEAMSv3.0 requires defining a water flow sequence type (*FLGSEQ*). Parameters related to slopes, slope-lengths and drainage areas were estimated as already explained (see Fig. 3).

An upper feasible application efficiency of 95% as well as a normally distributed fraction of the pesticide effectively applied to leaves (*FOLFRC*) were assumed (*SOILFRC* = *0.95-FOLFRC*). *FOLFRC* was made an increasing function of *LAI* to account for the decreasing probability of the pesticide to reach the soil as it is covered by increasing numbers of leaf layers. The timing of the pesticide applications was scheduled like in the base model run. The application rate (*APP. RATE*) was made a linear (uniform random) function of the crop leaf area index in order to account for the farmers' practice to adjust the amount of pesticide applied based on the age and size of citrus trees.

2.7. Output variables and regression analysis

The selected model output variables were the total mass of each pesticide lost from the area of application (runoff + sediment erosion + percolation) at the end of each of 3-year cultivation periods. The MC-GLEAMSv3.0 combined routines were run 10000 times and a post-processing subroutine was written to capture both selected MC-randomized input parameters and output control variables at each run. The vectors (size = 10000) describing MC-input/output were re-scaled to the [1–10] interval to facilitate the interpretation of a sensitivity analysis performed through stepwise linear regression (SPSS for Windows v7.5.1, SPSS Inc., Chicago, US) predictors of the form

$$y_i = a_{i1}x_1 + a_{i2}x_2 + \ldots + a_{ij}x_j, \tag{1}$$

where y_i ($i = 1,..,N$), is the total loss of pesticide and N is the total number of pesticides tested and j is the number of input variables selected by the stepwise procedure. Because of variable scaling, the a_{ij} are a measure of the sensitivity of the response variables y_i to a unit variation in the input variables x_{ij}, and $\Sigma_i a_{ij} \leqslant 1.0$. In selecting the x_{ij} through the stepwise procedure, only those are included in the sensitivity model that would increase its F-value probability at $p \leqslant 0.05$ significance level, and are deleted if they decrease the same at $p \leqslant 0.10$.

3. Results

3.1. Model run of modal case

The simulated daily pesticide concentrations in soils show peak values after dates of pesticide application, followed by a variable decline caused by wash-off during subsequent rain events (runoff + erosion + percolation) and pesticide decay (Fig. 5). Concentration declines also occur during mid-winter periods when pesticide applications are interrupted for about 60 days during crop low-growth season. Average concentration values are consistent with those obtained for the same crop and application rates based on pesticide fugacity estimates (Ares, 2004).

3.2. Sensitivity to management and environmental parameters

Fifteen un-correlated parameters were selected as significant through the stepwise regression procedure (Fig. 6). In this figure, the range ±1/15 along the y-axis separates those input parameters that produce a change in the model output over-proportional respect to their participation in the MC-shell (hyper-influential parameters). The directions of influence are either positive (higher parameter value – higher pesticide loss) as in *CN2, CLAY1, LAI* and *SATK1* or negative as in *FOLFRC*. The behavior of individual pesticides departs in some cases from the above average pattern (Fig. 7). The condition of the soil surface as described by the *CN2*-Curve-No. factor is a highly influential factor accounting for as much as 63-68% of the total loss of Carbendazem-2-4-D and 8% of Glyphosate. The efficiency of pesticide application

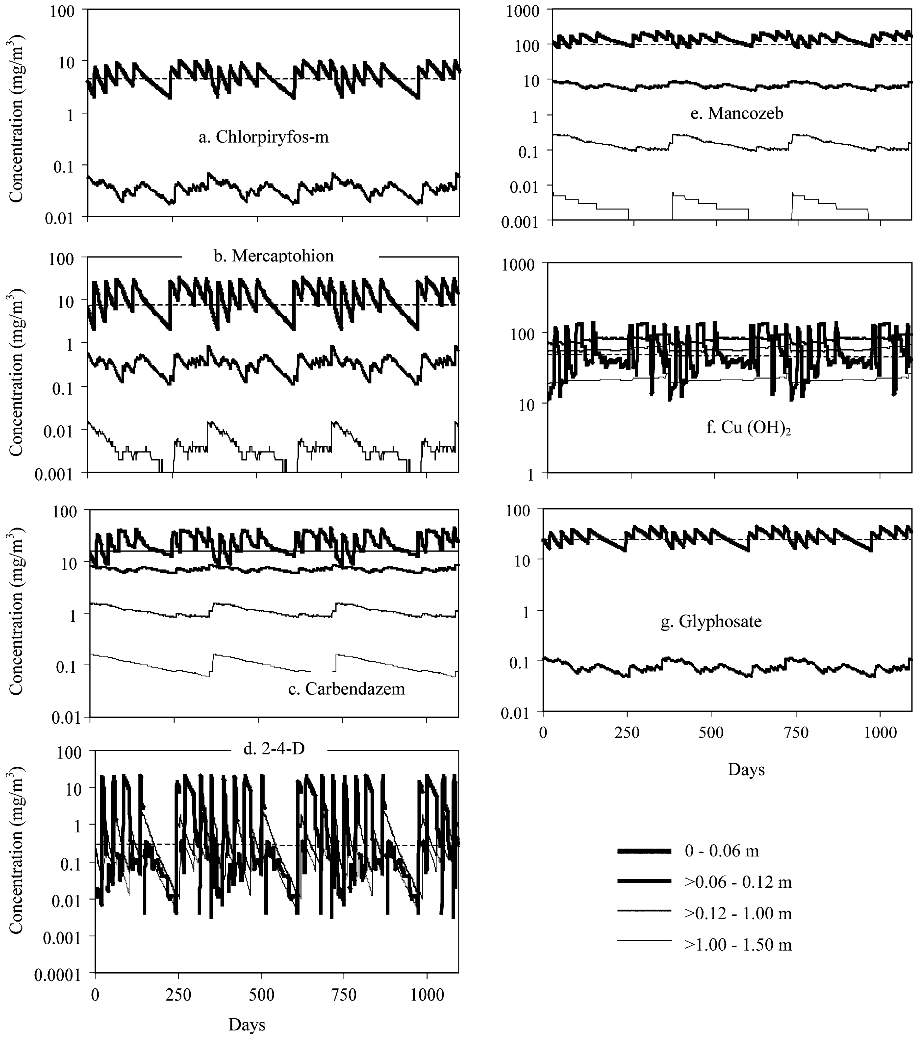


Fig. 5. Pesticide concentrations at various soil depths during three cropping years as estimated with GLEAMSV3.0 (base run).

as measured through the *FOLFRAC* parameter is highly influential in the cases of Chlorpyrifos, Carbendazem and Mancozeb. The *LAI* parameter is influential to Chlorpyrifos and Carbendazem losses.

4. Discussion

As with respect to our objective of formulating working hypothesis to improve pesticide management and reduce losses to the environment, some alternatives can

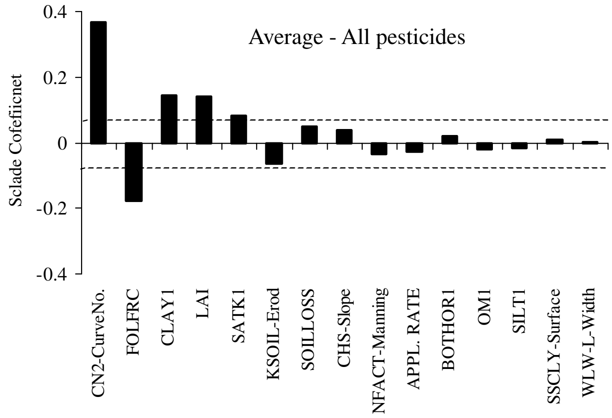


Fig. 6. Average values ($\bar{a}_j$) of coefficients of stepwise regression equations of the type: $y = \bar{a}_1x_1 + \bar{a}_2x_2 + \ldots + \bar{a}_jx_j$, ($y$: scaled pesticide loss; x_j: scaled input parameter; $j = 1,\ldots,15$) fitted to 10,000 MC-simulations with GLEAMSv3.0 ($p \leqslant 0.05$). The dotted lines indicate the boundary $\pm 1/15 = \pm 0.066$, corresponding to input parameters producing an over-proportional change in the model output (hyper-influential parameter).

be formulated. Citrus growers could reduce pesticide losses by applying agronomic practices that would change the roughness-contouring of the soil surface or its vegetation cover under the crop canopy (i.e., the *CN2* curve number, thus reducing the impact of water erosion on soils). A further potential area for improvement is with reference to *FOLFRAC*, the fraction of the applied pesticide that contacts the plant foliage. This can be improved through carefully devised spraying techniques, including adequate selection of the spraying equipment, avoiding pesticide application during unfavorable (windy, rainy) climate conditions and adequate formulation of the pesticide solutions, including the use of surfactants.

Our results also show that in these subtropical environments increasing the crop *LAI* would be expected to increase the losses of some pesticides like chlorpyrifos, 2-4-D, mancozeb and most notably carbendazem. This effect is probably caused by the frequent occurrence of intense precipitation events and consequent pesticide wash-off from plant leaves (a process included in the GLEAMS model), and constitutes a rather unfavorable sensitivity configuration. Crop *LAI* is a key management factor of crop production, and finding a compromise between optimum pesticide use and crop yield exceeds the scope of our study and might require further research. *LAI* could be manipulated in citrus through changes in plant spacing. Although citrus is a perennial crop and changing the plant spacing is not possible in most established plots, it could be modified in cases when conditions make it possible or in planning new crops.

Adequate corrective actions can also be applied to modify the relative amount of clay (*CLAY1*) and saturated hydraulic conductivity of the upper soil profile (*SATK1*), or due attention to these can be applied at the time of site selection to start new crops. Ranking individual crop fields with respect to these factors by entering

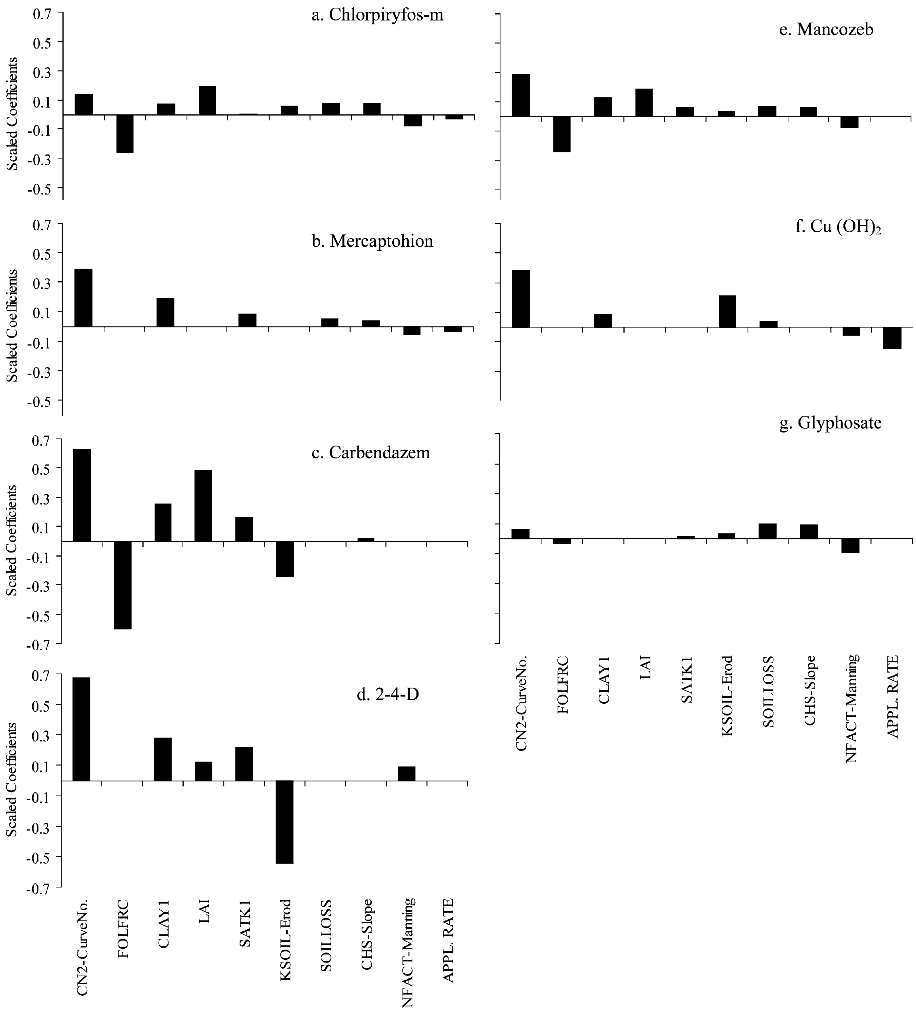


Fig. 7. Values of a_i coefficients of stepwise regression equations of the type: $y_i = a_{i1x1} + a_{i2}x_2 + \ldots + a_ix_j$, ($y_i$: scaled 'i' pesticide loss; x_j: scaled input parameter; only $j = 1,\ldots,10$ shown for graph simplicity) fitted to 10000 MC-simulations with GLEAMSv3.0 ($p \leqslant 0.05$) discriminated by pesticide.

pertinent local values in Eq. 1 can serve the purpose of selecting field cases for improving pesticide use and pesticide loss reduction.

Glyphosate deserves a separate comment because their losses proved to be relatively insensitive to all management and climate-soil related parameters that showed some relevance in the case of other pesticides. This type of behavior might represent a paradigm for selecting pesticides in this and similar environments where climate fluctuations and logistic-economic circumstances not related to the protection of the environment would interfere with motivated management options aimed to reduce pesticide losses to the environment.

It is also of interest to compare GLEAMS' sensitivities observed in sub-tropical environments with those observed in other climate regimes, where models with the same structural algorithms as GLEAMS have been tested. These studies identified various influential parameters, including the timing of pesticide application respect to rainfall occurrence and intensity, the partition with organic carbon in the soil and pesticide half-life (Leonard et al., 1987, 1992;Truman and Leonard, 1991). Lane and Ferreira (1980) identified rainfall as highly relevant in the case of weakly sorbed pesticides as well as application rate and runoff yield. Runoff curve number, porosity, field capacity, application rate and soil half-life were found as influential by Knisel (1993), while Zacharias and Heatwole (1994) found output sensitiveness to wilting point and leaf area index, but only minor sensitivity to curve number and field capacity. Ma et al. (1998, 2000) identified curve number, soil water content at field capacity and wilting point as influential parameters.

Some of the above results are not consistent among themselves or with the sensitivities we found in the subtropical environment of Misiones. The runoff curve number *(CN2)* seems to be a major agreement and our study also shows coincidence with those indicating leaf area index (*LAI*) as influential, depending on the particular pesticide considered. Other reported influential parameters like total rainfall, application rate, runoff yield, soil half life and wilting point were not identified as relevant in our case. The application rate was included in the independent shell but proved not relevant in our case, probably because of its partial dependence on the foliar area of the crop. Although not yet reported in previous studies, we found the fraction of pesticide effectively applied to leaves (*FOLFRAC*), the clay content of the upper soil layer (*CLAY1*) and its conductivity at saturation (*SATK1*) as highly influential. This latter might be homologous to the reported sensitivity to porosity in some cases (Knisel, 1993), but although porosity was explicitly considered in our MC-shell, it was discarded as non independent by the stepwise regression routine. Also, we found the soil erodibility factor (*KSOIL-Erod*) as significantly influential in carbendazem, 2-4-D and $Cu(OH)_2$ losses, a trend that might be related to the predominance of erosion-prone soils in the tested environments.

Some additional issues related to methodological aspects also arise. In previous studies on the sensitivity of pesticide models (Carbone et al., 2002; Havens et al., 2002), expert knowledge was applied to the pre-selection of "most influential" input parameters and this is probably a quite acceptable procedure at the stage of improving the model formulation and modeling research. However, it should be noted that the sensitivity of pesticide models depends on the subset of parameters selected for testing and the probability distribution functions assigned to them. This prompts the concept that the variables in the sensitivity shell and their associated distributions should be selected according to the specific purpose in using the pesticide model. In the case here presented, it seems appropriate not to include all possible combinations of parameters in model testing but instead restricting the search to landscape-crop-management related patterns of variation. Also, it seems relevant to orient the selection of parameters to be included in the MC-sampling to those that would represent management-amenable features at specific agricultural system and environmental conditions.

Landscape analysis techniques used in this study allowed estimating conditional PDFs relevant to pesticide fate prediction, so that no "fictitious case" is included in model simulations. This approach seems conceptually preferable to subjective selection of the sensitivity shell or imposing arbitrary variation ranges to model parameters.

Normalization in reporting sensitivity results of pesticide models also seems convenient. Some used formats in the past relate amounts of change (i.e., 10–100, etc.) to percentages of output change (Leonard et al., 1987). In other cases, n-fold changes in input parameters were related to similarly expressed variations in model output (Truman and Leonard, 1991). Also, sensitivity results were expressed in conditional terms, as referred to some part of the range of variation of input variables (Knisel, 1993). Other alternatives were single parameter variance (Walker et al., 1995), Placket-Burman matrices (Wolt et al., 2002) and Fourier perturbation analysis (McRae et al., 1982). This variability in structuring the analysis of sensitivity of pesticide models introduces difficulties in drawing comparisons among the reported results and their relative meaning. It would probably contribute to draw pertinent comparisons among studies on a same or different pesticide models, if some basic common procedure would be always included along with the used technique.

The approach used in this study seems convenient in various respects. Range equalization (1 to 10 would be a reasonable choice) of the input parameter values is convenient in order to compare the relative effects of variously scaled parameters. The discrimination of statistical independence by standard regression procedures results in convenient expressions of the change in the output produced by a unitary change in non-correlated input parameters. The resulting coefficients expressing sensitivities could in this way be compared among studies, sites, purposes and models. The procedure also yields confidence intervals for the sensitivity estimates, a valuable alternative when comparing the performance of a same model in different scenarios. Last, the definition of confidence intervals allows discriminating (hyper) influential parameters that modify the output to an extent that significantly exceeds that corresponding to their proportional participation in the sensitivity shell.

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References

Ares, J., 2004. Estimating pesticide environmental risk scores with land use data and fugacity equilibrium models in Misiones, Argentina. Agr. Ecosyst. Environ. 103, 45–48.

Buchter, B., 1989. Correlation of Freundlich Kd and retention parameters with soils and elements. Soil Sci. 148, 370–379.

Carbone, J.P., Havens, P.L., Warren-Hicks, W., 2002. Validation of pesticide root-zone model 3.12. employing uncertainty analysis. Environ. Toxicol. Chem. 21, 1578–1590.

Cohen, S., Fuchs, M., 1987. The distribution of leaf area, radiation, photosynthesis and transpiration in a Shamouthi orange hedgerow orchard. Agr. Forest Meteor. 40, 123–144.

de Paz, J., Ramos, C., 2001. The use of a GIS-N model system to assess nitrate leaching in agricultural areas. Acta Hort. 563, 225–231.

Dubus, I.G., Janssen, P.H.M., 2003. Issues of replicability in Monte Carlo modeling: a case study with a pesticide leaching model. Environ. Toxicol. Chem. 22, 3081–3087.

Duda, R.O., Hart, P.E., Stork, D.G., 2001. Pattern Classification. Wiley-Interscience, New York.

Eastman, J.R., 2001. Guide to GIS and Image Processing. Clark Labs, Worcester.

García, M., Chuvieco, E., 2003. Assessment of the potential of the SAC-C multispectral medium resolution scanner (MMRS) imagery for mapping burned areas. In: Proceedings of the 4th International Workshop on Remote Sensing and GIS Applications to Forest Fire Management: Innovative Concepts and Methods in Fire Danger Estimation. European Association of Remote Sensing Laboratories and Global Observation of Forest and Land Cover Dynamics (GOFC-GOLD). Ghent, June 5–7 June, 2003..

Gordon, J., Shortliffe, E.H., 1985. A method for managing evidential reasoning in a hierarchical hypothesis space. Artif. Intel. 26, 323–357.

Havens, P.L., Carbone, J.P., Warren-Hicks, W., Fouch, M.A., 2002. Development of a Monte Carlo sampling shell for the pesticide root zone model and its application by the Federal Insecticide, Fungicide and Rodenticide Act environmental modeling validation task force. Environ. Toxicol. Chem. 21, 1566–1569.

Knisel, W.G., 1993. GLEAMS: Groundwater Loading Effects of Agricultural Management Systems, Ver 2.10. University of Georgia Coastal Plain Experiment Station, Tifton, GA, USA.

Knisel, W.G., Davis, F.M., 2000. Groundwater Loading Effects of Agricultural Management Systems. Version 3.0. Publication No. SEWRL-WGK/FMD-050199, revised 081500, Washington..

Lane, L.J., Ferreira, V.A., 1980. Sensitivity analysis. In: Knisel, W.G. (Ed.), CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. US Department of Agriculture, Southwest Watershed Research Center, Report 26. Tucson, Arizona..

Leonard, R.A., Knisel, W.G., Still, D.A., 1987. GLEAMS: ground loading effects of agricultural management systems. Trans. ASAE 30, 1403–1418.

Leonard, R.A., Truman, C.C., Knisel, W.G., Davis, F.M., 1992. Pesticide runoff simulations: annual means vs. event extremes. Weed Technol. 6, 725–730.

Ligier, H.D., Mattelo, H.R., Polo, H.L., Rosso, J.R., 1990. Misiones. In: Secretaría de Agricultura, Ganadería y Pesca (Ed.), Atlas de Suelos de la República Argentina. Escala 1:500000 y 1:100000. Instituto Nacional de Tecnología Agropecuaria, Buenos Aires, pp. 121–139..

Ma, Q.L., Wauchope, R.D., Hook, J.E., Johnson, A.W., Truman, C.C., Dowler, C.C., Gascho, G.J., Davis, J.G., Sumner, H.R., Chandler, L.C., 1998. GLEAMS, Opus, and PRZM2 model-predicted versus measured water runoff from a coastal plain loamy sand. Trans. SAE 41, 77–88.

Ma, Q.L., Hook, J.E., Wauchope, R.D., Dowler, C.C., Johnson, A.W., Davis, J.G., Gascho, G.J., Truman, C.C., Sumner, H.R., Chandler, L.C., 2000. GLEAMS, Opus, PRZM2, and PRZM3 simulations compared with measured atrazine runoff. Soil Sci. Soc. Am. J. 64, 2070–2079.

McRae, G.J., Tilden, J.W., Seinfeld, J.H., 1982. Global sensitivity analysis. A computational implementation of the Fourier amplitude sensitivity test (FAST). Comput. Chem. Eng. 6, 15–25.

Monmonier, M., 1982. Computer-Assisted Cartography: Principles and Prospects. Prentice-Hall Inc., Englewood Cliffs.

Perry, R.H., Green, D.W., 1973. Perry's Chemical Engineering Handbook. McGRaw Hill, New York.

Pinti, B., Verstraete, M., 1992. GEMI: a non-linear index to monitor global vegetation from satellites. Vegetatio 101, 15–20.
SAGPyA-Secretaría de Agricultura, Ganadería, Pesca y Alimentación, 2000. Proyecto de Fortalecimiento de los Servicios Fitosanitarios de la Prov. de Misiones. Documento Principal. SAGPyA, Buenos Aires..
Saxton, K.E., Rawls, K.W., Romberger, J.S., Papendick, R.I., 1986. Estimating generalized soil-water characteristics from texture. Soil Sci. Soc. Am. J. 50, 1031–1036.
Searing, M.L., Shirmohammadi, A., Magette, W.L., 1995. Utilizing GLEAMS model to prescribe best management practices for critical areas of a watershed identified using GIS. ASAE Paper No. 95-2402, ASAE, St. Joseph, Misouri..
Truman, C.C., Leonard, R.A., 1991. Effects of pesticide, soil, and rainfall characteristics on potential pesticide loss by percolation. A GLEAMS simulation. Trans. ASAE 34, 2461–2468.
Walker, A., Calvet, R., Del Re, A.A.M., Pestemer, W., Hollis, J.M., 1995. Evaluation and Improvement of Mathematical Models of Pesticide Mobility in Soils and Assessment of their Potential to Predict Contamination of Water Systems. Blackwell Wissenschafts-Verlag, Berlin, Germany.
Warren-Hicks, W., Carbone, J.P., Havens, P.L., 2002. Using Monte Carlo techniques to judge model-prediction accuracy: validation of the pesticide root zone model 3.12. Environ. Toxicol. Chem. 21, 1570–1577.
Wedwick, S., Lakhani, B., Stone, J., Waller, P., Ariola, J., 2001. Development and sensitivity analysis of the GLEAMS-IR model. Trans. ASAE 44, 1095–1104.
Wolt, J., Singh, P., Cryer, S., Lin, J., 2002. Sensitivity analysis for validating expert opinion as to ideal data set criteria for transport modeling. Environ. Toxicol. Chem. 21, 1558–1565.
Yulianti, J.S., Lence, B.J., Johnson, G.V., Takyi, A.K., 1999. Non-point source water quality management under input information uncertainty. J. Environ. Manag. 55, 199–217.
Zacharias, S., Heatwole, C.D., 1994. Evaluation of GLEAMS and PRZM for predicting pesticide leaching under field conditions. Trans. ASAE 37, 439–451.