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Simulating human and environmental exposure from hand-held knapsack pesticide application: Be-WetSpa-Pest, an integrative, spatially explicit modeling approach

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Abstract

This paper presents an integrative and spatially explicit modeling approach for analyzing human and environmental exposure from pesticide application of smallholders in the potato producing Andean region in Colombia. The modeling approach fulfills the following criteria: (i) it includes environmental and human compartments; (ii) it contains a behavioral decision-making model for estimating the effect of policies on pesticide flows to humans and the environment; (iii) it is spatially explicit; and (iv) it is modular and easily expandable to include additional modules, crops or technologies. The model was calibrated and validated for the Vereda La Hoya and was used to explore the effect of different policy measures in the region. The model has moderate data requirements and can be adapted relatively easy to other regions in developing countries with similar conditions.

Keywords: integrative model, pesticide, exposure, environment, behavior, hydrology, developing countries

Introduction

World-wide pesticide use in crop production has constantly been increasing since the 1950s in total amount and in quantities per unit area [1,2]. Whereas in developed countries, mostly herbicides are applied and the environmental impacts, e.g., fish toxicity, soil damage, are of major concern [3-6] in developing countries, the bulk of pesticides used are insecticides and fungicides and human mortality and morbidity due to exposure to pesticides has become a concern as it significantly affects the livelihood of small farmers [7,8].

Several tools have been developed to assess and reduce the impact of pesticides on the environment and on human health [9]. Of special interest in our case is the development and use of models. A first string of research develops environmental pesticide fate models. They analyze the distribution of pesticides within the environment, including plant, soil, water and in some cases through air (drift) (PEARL [10], CESMOS, BASINS (HSPF) ,[11]SWAT [12], Wet_hydro [13], etc.). A particular group of models studies explicitly the contamination of water bodies. Models in this category are for example DRIPS, EXAMS, PIRANHA a/b/c (see [14] for a review). Other models, such as empirical curves, focus on pesticide airborne or drift deposition and were developed in the temperate region for terrestrial mechanized boom sprayers [15-19]. Some of these models perform optimally after calibration for the case of hand-held knapsack sprayers, mostly used in developing countries in the tropics, recently demonstrated by García-Santos et al. [20]. More sophisticate models focusing on pesticide exchange with the atmosphere after applied to soils and crops are dynamic and physically based [21].The most advanced model within pesticide emission models is the PestLCI model [22,23] and was developed for use in agricultural life cycle assessment following mechanized spray application at local scale [24]. As these models have all been developed for special needs and conditions of use, they differ in their spatial and temporal scales, time step, spatially explicitness, processes modeled, data requirements, complexity and output (see [14] for a review). Furthermore, most of these models have large data requirements and have never been applied in developing countries [25] and none of these models includes potential human exposure of the applicators as an output.

Within a second string of research, tools and models have been developed to assess human exposure to pesticide use. The tools range from qualitative assessment of human exposure, focusing mostly on dermal exposure (e.g., DERM [26]; EASE [27]; PHED [28]; COSHH [29]; DREAM [30]; RISKOFDERM [31]; STOFENMANAGER [32]; see [33,34] for a review), to sophisticated quantitative simulation models of pesticide emission in the air (Plume Model "Gaussian Plume" [35]; Gaussian Diffusion Model (GDM) [36]; Model for Risk assessment of pesticide drift damage [37]; One-Box Model [38]). These models focus specifically on human exposure and do not include environmental effects. The only tools in which both the environment and human health issues are included are empirical studies [39] and indicator based assessments (see [40] for a review). However, these assessment methods are usually neither dynamic nor spatially explicit e.g. accumulation issues, feedbacks and self-organization processes as part of the system dynamics are neglected. Furthermore, another disadvantage of empirical point-based static approaches is that the evaluation of probability is usually insufficiently considered [41] and key parameters might be not considered since they were developed in different contexts [42].

A third string of models combines agricultural production models (including pesticide use and to some extent environmental fate models) with economic models; an area where there has been significant progress in the last years (see [43] for a review; [44,45]). The integration of models ranges from linear programming models to spatially explicit multiple scales and multiple goal models [46,47]. A few models analyze the effect of environmental degradation, e.g. erosion, water contamination on farmers' income and on the economic system at a regional level (e.g., ECECMOD [48]; and SAM [49]). The trade-off model [50] is the only integrative model that has been applied to pesticide management of potatoes in the Andes Region. It combines bio-physical models with econometric-process simulation models and provides an integrated analysis of tradeoffs between economic and environmental indicators. However, it has been found that farmers decision-making is often affected by parameters other than economic ones such as norms and traditions [51,52] and thus behavioral models are required which, on the one hand, simulate farmers' behavior and estimate the impacts of policies on pesticide use and, on the other hand, can be linked to spatially explicit pesticide models estimating the impact of behavioral change on human and environmental exposure. Finally, most models have high data requirements that cannot be met in developing countries and thus less data demanding models are required [40].

This study contributes to the development of integrated models in the area of pesticide management. The modeling approach, Be-WetSpa-Pest, (i) integrates a hydrological model with an extended pesticide emission model considering environmental and human compartments; (ii) is coupled to a behavioral model, for estimating the effect of different policies on farmers pest control behavior, affecting pesticide distribution in the environment and onto the applicator; and (iii) has already been applied to Vereda La Hoya, Colombia, a region with low data availability.

We combine a farmer behavioural model [53], with a spatially explicit hydrology model, WetSpa [54], and a pesticide emission model, PestLCI [22]. We assess the potential human and environmental fate of pesticides due to adoption of different policies in low mechanized cultivation of potato in the Colombian Andes (a tropical region).

Methods

Be-WetSpa-Pest[1]: Model structure. Figure 1 presents the basic model structure composed of input data, core model processing and the output data. The strength of the Be-WetSpa-Pest is its modular structure, preferred over a fully integrated model approach as it facilitates the use, inclusion and adaptation of disciplinary models in the shape of modules, i.e. hydrological, fate and behavioral model, to different study areas (see also [50]), additional crops, pesticides and technologies.

<Figure 1>

Input data. To run the model four types of data are needed (Fig. 1 and 2 in Database box; Table 1 in 01_Supporting information): "global parameters" as parameters required for the hydrological WetSpa model and pesticide emission PestLCI model, "climate data", i.e., representative meteorological data of the catchment, "spatial metadata", i.e., spatially explicit land use, catchment, weather station and appropriation data, "pesticide data", i.e., physical and chemical properties of applied pesticides, and "external socio-economic factors", i.e., policies and crop rotation. The input data are stored in form of different GIS layers (Fig.2 File system box; Table 3 in 01_Supporting information). Ownership information was entered in GIS based on the latest Cadastral map [55]. Physical and chemical properties of applied pesticides within "pesticide data" were obtained from the PestLCI database and own empirical field experiments in similar soils [56,57].

<Figure 2>

Model processing. The core model, so-called Be-WetSpa-Pest model, is composed of a behavioral model and the WetSpa-Pest model. The "Behavioral model" predicts pesticide type (most prominent three fungicides and insecticides for the case study), amount applied, and application frequency per farmer and plot in the study area [53]: this information is used in the pesticide emission's model as total pesticide applied (P_A, in equation 1).

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[1]Beta version available upon request.

A set of influencing factors contributes in determining the probability of a farmer to adopt a fungicide and insecticide application type respectively (see section 3 of 02_supporting information). Concerning fungicides, the influencing factors are training delivered by pesticide producing companies, the proportion of household income coming from agriculture, the sense of compliance with the prescriptive social norm (i.e. other farmers recommendations), the plot area, and being member of a farmer cooperative. Concerning insecticides, the influencing factors are farmer's educational level, the presence of significant sources of non-agricultural income for the household, training delivered by pesticide producing companies, and the plot area ([53] and 02_supporting information). The default values of these factors (i.e. those used in the baseline scenario) in WetSpa-Pest correspond to those observed in Vereda La Hoya [52,53].

The model allows for modifying the value of selected factors for each farmer, thus simulating different types of interventions on pesticide use in the area. Interventions that WetSpa-Pest allows to be simulated are: i) intensification of training delivered by pesticide producing companies; ii) organization of farmers in a cooperative; iii) modification of household non-agricultural income sources; iv) increase/decrease of farmer sense of compliance with the prescriptive social norm. It has to be noted that the policies intervene on those farmers who in the baseline scenario did not already participate in a training program or who were not intervened. In the behavioral model, a farmer can adopt one among three different fungicide and insecticide application types that correspond to decreasing input effectiveness levels [53]. The application types differ in terms of i) intensity of application (i.e. quantity of active ingredients per unit of surface), ii) number of applications per agricultural cycle, and iii) class of active ingredients applied, in particular with respect to the share of carbamates and pyrethoids over the total quantity of fungicide and insecticide ([53] and Table 5 in 01_Supporting information). Furthermore there is the option to use the option "crop rotation" based on [58,59].

The behavioural model is coupled to the WetSpa-Pest model and provides the interface for entering and assessing policy recommendations. Application frequencies (i.e. average number of pesticide application per phase of agricultural cycle) is also associated to the adoption of a fungicide and of an insecticide application type, respectively. This information is used to determine application dates, which can be distributed either randomly (using the math.random algorithm in which the values are chosen pseudorandomly with approximately uniform distribution from the range [0.0 - 1.0]) or evenly within each phase of the agricultural cycle excluding Sundays and days with rain (i.e. conditions by which farmers from the study area do not apply pesticides). In addition, the first application date in a cycle must be on a Tuesday (on even applications), and the application time must be between 06:00 and 17:00, i.e. the time in which farmers usually work in the fields (see section 4.2 of 02_Supporting information). The empirical data on pesticide use per farmer and plot proceed from the survey of 25% of the registered farmers in the catchment area [52]. Therefore, an algorithm was developed to extrapolate the data from these known data plots to all other agricultural plots in the study area. For details on the extrapolation algorithm see section 5 of 02_Supporting information.

The second part of Be-WetSpa-Pest model is the WetSpa-Pest model. WetSpa-Pest is a fully distributed, spatially explicit hydrology and emission pesticide model based on the WetSpa model by Liu and Smedt [54] and the here modified PestLCI model [22], respectively. The model WetSpa is a GIS-based distributed hydrological model for flood prediction and water balance simulation on a catchment scale (for more details on the water flows on a cell basis see [54]). It was developed by the Free University of Brussels and can be downloaded for free (http://www.vub.ac.be/WetSpa/). The pesticide emission model PestLCI was developed in Denmark by Birkved and Hauschild [22] (updated version in [23]) to provide information for the estimation of pesticide mass in the environment (air, surface water and groundwater) outside of the sprayed field after aircraft, boom spray (pull tractor) or soil injection application techniques to be included in life cycle assessment. Its modular structure allows adaptation to conditions for different regions and agricultural practices and techniques. A human exposure component was added and drift fraction was modified for hand-held spray pest application (more details below).

Thus, Wetspa-Pest simulates simultaneously the dynamics and balances of water, energy and pesticide on a grid (cell) basis at catchment scale. It uses as input data the type, amount, and frequency of pesticides use per plot estimated based with the behavioural model [53]. As in WetSpa, WetSpa-Pest simulates simultaneously water processes i.e. snow processes (freezing and melting), canopy interception and potential evapotranspiration, infiltration, percolation, surface runoff generation, interflow, groundwater flow and river routing, pesticide flows distribution into the compartments air, water, soil and canopy, based on the modified PestLCI model and farmer's exposure fraction based on own field experiments [60].

In our study, each cell (30 x 30 m) is a unit process (technosphere in life cycle assessment studies), equivalent to an agricultural field where only one crop grows, which is cultivated by one farmer with spatially uniform pesticide application. The cell is vertically divided into different environmental compartments i.e., air (100 m vertical), canopy, soil (soil surface, soil matrix and groundwater) (1 m soil depth), as in PestLCI 2.0 [23] and additionally includes a human compartment i.e., applicator. When a pesticide leaves the unit process (cell), it is considered an emission. The model takes into account emissions to air, surface water and groundwater compartment like in PestLCI and additionally emissions to soils outside of the cell as pesticide soil deposition from drift, as harvest (leaf uptake) and as applicator (human exposure).

The primary pesticide distribution processes are those taking place during pesticide spray application as described by the equation (1):

$$P_A = (P_V + P_D + P_H + P_L + P_S)\, P_A/100 \qquad (1)$$

where P_A is the total pesticide (active ingredient) applied (kg active ingredient/ha), P_V is the pesticide fraction which stays in the air of the plot (%), P_D is the pesticide drifted by wind out of the sprayed plot (%), P_H is the pesticide that reaches the applicator (human exposure) (%), P_L is the pesticide fraction deposited on the leaves (canopy) (%) and P_S is the pesticide directly reaching the soil (%).

Total pesticide applied (P_A): The quantity (kg/ha) and type of active ingredients applied in a plot, and the frequency of application are determined through the behavioral model (see above) developed by Feola and Binder [52,53].

Pesticide staying in the air (P_V): The value for the pesticide staying in the air depends on the type of pesticide and meteorological conditions of the area. It can be entered into the model as a specific fixed value. In the case of Vereda La Hoya the value of 1 % was used given the measurements in the field [59].

Pesticide drifted by wind (P_D): Hand-held spray is not a considered technique in the PestLCI or PestLCI 2.0. For the case of hand-held spray inpotato production, it is found that drift is higher as compared to conventional boom spray with tractor [61] and therefore the here modified PestLCI includes two possibilities a fix drift fraction of 3.1% of the applied dose as derived from García-Santos et al. [62] or calculation of drift for the first 20 m outside the plot in function of distance through the optimized IMAG drift calculator (v 1.1) by Holterman and Zande [16] (in PestLCI v2) after García-Santos et al. [61] (optimized parameters: a = 29, b = -6.8, c = 18.35, d = -0.44). Other equations in function of wind speed may reflect a more realistic scenario in cases where spray is conducted under wind conditions above 2 m s^{-1}, available in García-Santos et al. [61]. This could be added into the model structure.

Pesticide reaching the human (P_H) (not in PestLCI 2.0): P_H is the fraction of the pesticide reaching the farmer's clothes and is calculated by using a fixed fraction of 1% of the total pesticide derived from empirical measurements [60]. The type of protection equipment used determines the final exposure of the farmers [60]. In the case we applied the model, Vereda La Hoya, farmers use gummy boots, long trousers and a T-shirt covered by a "ruana" or "poncho".

Pesticide fraction deposited on the leaves (canopy) P_L: P_L in Eq. 3 depends, besides the amount of pesticide drifted away and the amount landing on the applicator, on the leaf area covered and thus on the growth stage of the plant,

$$P_L = (P_A - P_H - P_D - P_V) * v_i \quad (3)$$

where v_i is the interception fraction and represents the growth stage of the plant [63].

Pesticide reaching directly the soil (P_S): P_S is calculated as the balance from the total amount of pesticide applied and the pesticide reaching the other compartments,

$$P_S = P_A - P_V - P_D - P_H - P_L \quad (4)$$

After the plot is treated, the applied pesticide is redistributed in the environment and degraded. The secondary modelled processes by WetSpa-Pest after the pesticide application are infiltration into soil, percolation into the groundwater (WestSpa model), and pesticide outflow of the watershed through surface runoff (fraction of pesticide in the top soil liquid phase) and groundwater flow (fraction of pesticide in the soil matrix liquid phase) (modified PestLCI) (see equations in 03_Supporting information and coefficients in 01_Supporting information Table 2). Pesticide loss through macropore flow and tillage (considered in PestLCI 2.0) is not modelled but could be incorporated into the model.

Output data. The output data is composed first of hydrological times series, including infiltration, percolation, and evaporation, and surface runoff. The data is used to calibrate the WetSpa part of the model. Second, spatially explicit pesticide concentration data onto the applicator, the crop (as harvest), soil surface, soil matrix, surface runoff and groundwater is generated. Furthermore, for a specific plot, the same information can be obtained as time series (Fig. 2).

Case study. Be-WetSpa-Pest was implemented in a typical Andean mountainous region, the department ("Departamento") of Boyacá, which contributes to ca. 26% of the national potato production and to 45% at regional level despite its low productivity, and its land tenants are mainly smallholders (95% of the workforce) [20, 70]. The same area of study has been focus of recent studies on human and environmental exposure from hand-held knapsack pesticide applications [20,39,40,44,45, 52,53,60,61,62,64,69]. The study area Vereda La Hoya has 840 ha and is located in the district La Hoya of the community Tunja (Colombia) at a height of about 2800 to 3200 m a.s.l. It lies in the cold climate thermal floor zone, with a total mean annual rainfall of 620 ±20 mm. The area has prevailing south-east winds with average wind speed of 1.8 ±1.39 m s^{-1} and a maximum of 7.6 m s^{-1} (data from this study). Meteorological variables were registered every 15 min for 3 years, from October 2008 until October 2011, at 3 m above ground, using a low cost automatic meteorological station, Davis Vantage Pro-2, installed within the watershed because no representative weather information was found in the national net (IDEAM).

The moisture regime of the soil is ustic and soil texture according to US-Soil taxonomy is sandy loam as described by García-Santos and Keller-Forrer [64] and [65]. Average pH of the soil is 5.03 ± 0.31. Total organic carbon is 9.51 ± 3.93 % (Walcley Black method) and bulk density is 0.84 ± 0.1 gr cm^{-3}[64,66]; The seasonality of water discharge is caused mainly by variations in rainfall events in May and October, ranging from less than 10 l s^{-1} in pre-event situations to above 60 l s^{-1} during spring and autumn. Discharge regularly intermits during summer. Water flow at the outlet was measured using an ultrasonic Doppler sensor (Unidata STARFLOW) calibrated with a propeller. Measured water velocity was multiplied by the cross section to obtain water flow (l s^{-1}).

Orographic characterization of the catchment was obtained through a digital elevation model. A geographic information system (GIS) was used to store digitized land use representing the watershed characteristics with a grid of 100 x 100 m and to convert the information to raster [55].

Main crop production in Vereda La Hoya is potato. The catchment lies within the second highest potato producing region in Colombia, Boyacá, after Nariño [67]. In the region, mostly *solanum tuberosum spp* is produced. The potato cycle last about 6-7 months and the average yield is low with about 7 ton/ ha and cycle [53]. Farmers cultivate an average of 3 ha, which are subdivided into small plots, being to a large extent distant from each other within the catchment and most located on terrains, which are not appropriate for mechanization.

Pests are controlled through the application of insecticides and fungicides (see [53] for details) during the entire cycle using hand-held sprayers, lever-operated knapsack sprayer.

Model calibration and validation of the hydrological module. The hydrological module was calibrated following the principles of the guidelines for WetSpa calibration by Liu and Smedt [54]. First, a rough calibration was made separately for the WetSpa model using the stream flow data from the study area. Calibration data were from 4.9.2010 - 17.10.2010 and 28.10.2010 - 28.11.2010). These periods included a precipitation event with a return period of 25 years. The gap is due to missing discharge and meteorological data. Second the parameters: correction factor for evapotranspiration; surface runoff exponent; threshold rainfall intensity; interflow scaling factor, and baseflow recession coefficient were calibrated using the 3 months with highest rain intensity (September to November) during 2010 (see also [54]). Third, the hydro-meteorological data from 29.11.2010 to 19.12.2010 was used for validation of the model. To evaluate the goodness of fit of the modeled discharge during the calibration and validation period, we used five statistical criteria (Table 1): the model bias [54] which is the relative mean difference between predicted and observed stream flows (0 represents a perfect fit);

the Nash-Sutcliffe efficiency [68] cited in [54], which is used to evaluate how good the model simulates the stream flow (1 indicates a perfect fit); the RMSE (root mean square error); the Pearson coefficient of determination (R^2); and the standard error.

<Table 1>

Model validation of the pesticide module in soil. To validate the pesticide module of the WetSpa-Pest, we modeled the concentration in soil of an active ingredient used (i) widely and (ii) in high dosage in the study area. Chlorpyrifos corresponded to these characteristics and is used to protect the crop from three typical pests threatening the potato crop in the study area: the soil-dwelling larvae of the Andean weevil (Premnotrypes vorax), the late blight fungus (Phytophthora infestans) and the Guatemalan potato moth (Tecia solanivora) [53]. The crop cycle period extended from the 20th September until the 28th December 2009. The day and time of pesticide application, day of planting and day of harvest represent real conditions as reported by the farmer. Predicted concentrations were compared to previously measured concentrations in the same area [69]. The calculated concentrations in soil showed a high agreement with the measured values along the different stages of growth of potatoes with an r^2 of 0.82 (Figure 3). The modeled values lied to a large extent within the error margin of the measured concentrations.

<Figure 3>

Simulation scenarios. To show some of the results the model can generate, we used Be-WetSpa-Pest to simulate three scenarios, i.e. a “baseline scenario”, ‘training by companies’ and ‘cooperative’ respectively. The latter two were developed to exemplify how the model can be used to assess the effect of policies on pesticide use, and environmental and human exposure. We show the results for the use of the active ingredient Mancozeb, applied six times with different time spans in between the applications, from 20.07.2009 to 20.12.2009 for a specific field in the study area.

All scenarios simulate fungicide and insecticide application over 4 agricultural cycles of potato production (see Table 4 and Table 5 in 01_Supporting information). The first and second cycle correspond to a baseline scenario, in which self-reported pesticide application rates are used [53]. The initial values of parameters in the behavioral model (see section above) also correspond to observed values in the study area [53]. The third and fourth agricultural cycle served to run the “training by companies” and “cooperative” separately.

Results and discussion: application of the Be-WetSpa-Pest model

The baseline scenario. Figure 4 shows the simulation results for a specific plot of the active ingredient Mancozeb funguicide (C8H12MnN4S8Zn), an ethylenebisdithiocarbamate (CAS Number:8018-01-7). On the top X-Axis and the right Y-Axis, precipitation on the plot is depicted, on the lower X-Axis and the left Y-Axis, the concentration of Mancozeb is shown. The first application (20.8.2009) took place at the start of the growth phase. The amount of Mancozeb intersected by the canopy is low, a large share of the Mancozeb applied (about 83 %) end in the topsoil and some infiltration occurs when there is precipitation. In the larger growth stage (20.10.2009), the plant intercepts a higher percentage of the pesticide leading to a lower amount reaching the topsoil (up to a share of about 48% for plant and topsoil). The amount infiltrating through the topsoil to the soil is rather below <4% and is favored is by precipitation due to the wash off from canopy to topsoil and from topsoil to soil. The total amount of Mancozeb accumulated in the soil is low and zero at the end of the cycle. On contrary, the concentration in the topsoil decreases slowly and one could potentially encounter residues even when the next cycle starts. This is not only due to the application itself, but also to the withering and degradation of the vegetation stubbles after harvesting the potatoes.

<Figure 4>

Figure 5 shows the spatial distribution of the pesticide concentration in the watershed for Mancozeb at the end of the four simulated cycles (the same case as above). Red (Hotspots) are the plots with high Mancozeb concentrations (between 4-8 kg/ha), in the green plots no pesticides were applied at all. Hotspots of topsoil concentrations higher than 1 kg/ha can only be found in a few places, however some of them being close to a stream. The light green plots show the pesticide concentrations due to drift. On these plots no pesticides were applied but we could simulate low concentrations of Mancozeb. The contaminated plots are spatially interconnected, which is due to similar cultivation practices on neighboring plots and the drift of pesticides to neighboring plots.

<Figure 5>

Scenario analysis. In the policy scenario 'training by companies' we simulate the effect of a training program held by pesticide producing companies. We considered only the farmers who had no intervention in the baseline scenario. For these farmers, the introduction of the policy modifies the probability of adopting one of three fungicide and insecticide application types respectively. This potentially determines a variation (i.e. increase) of pesticide released into the environment. The results show a marginal increase in productivity, but a significant increase in fungicide and insecticide use ([53]). In the policy scenario 'cooperative' we simulate the effect of the participation of farmers in producer cooperatives. The results show that this scenario significantly improves the efficacy of insecticide use, that is, it reduces insecticide use rates [53].

Figure 6 shows the total amount of active ingredient of two fungicides and two insecticides applied in the total area during one cycle (140 days) for the baseline and the two scenarios mentioned above. Regarding the insecticides, Carbofuran and Permethrin, almost no differences can be found between the scenarios, implying that these policy measures will not be effective in reducing exposure to pesticides in the case studied. For the fungizides Mancozeb and Cymoxanil the training by pesticide producing companies significantly increases the amount of pesticides applied, whereas joining a cooperative reduces the amount of fungicides applied by almost 90%. This suggests that fostering cooperatives and providing training and production support through the cooperatives might be a good way forward to reduce the amount of fungicides applied. Even though this variable shad a strong estimated effect on fungicide use it was not significant for insecticides use and was therefore not included in the equation. That is, insecticide and fungicide use are determined by different sets of factors, and even when there is one factor that influences both pesticide and insecticide use (e.g. the proportion of household income coming from agriculture), the coefficient is not the same in both equations for the two behaviors (as estimated in the statistical models [53]). This indicates the necessity for a disaggregated behavioral analysis for pesticide use rather than an overall analysis looking at the amount of money spent on pesticides.

<Figure 6>

When looking at the spatial distribution of Mancozeb (Figures 7 a,b), the amount of hotspots (>1 kg/ha) increases in the case of the training scenario, whereas the areas, where pesticide amounts higher than 1kg/ha can be found in the topsoil is markedly reduced in the cooperative scenario. In particular, the concentration of Mancozeb in the areas close to the river is reduced. This result reflects the necessity of a spatially explicit analysis (see also [50]) to provide decision support for reducing surface water contamination by decreasing the pesticide concentration on plots close to surface water areas.

<Figure 7>

Model use recommendations and further model developments.

This paper presented Be-WetSpa-Pest, a simulation model that (i) integrates a hydrological model with an extended pesticide emission model considering environmental and human compartments; and (ii) is coupled to a behavioral model, for estimating the effect of different policies on farmers' pest control behavior, affecting pesticide distribution in the environment and onto the applicator. The model was calibrated and validated for the case of Vereda La Hoya in Colombia and provided valuable results on the effect of policies on humans and environmental exposure to pesticides. We suggest the model to be applicable for similar cases in developing countries, where there is low data availability. However, we recommend, for the environmental part, to measure the key input variables for climate data like daily precipitation and temperature from a nearby station, and to obtain a DEM of the area to be studied for the spatial data.

It was shown that changes in farmers´ behavior play a significant role for environmental and human exposure and that policies affect fungicide and insecticide use in a different way. To apply Be-WetSpa-Pest to other regions, thus, we consider that (i) the behavioral model should be validated. In a similar cultural background as the case study, we expect that the influencing factors might be the same, even though their impact (i.e. the estimated coefficient in the deterministic equation) might differ. In other cultural contexts, it is likely that not only the influencing factors' estimated effects, but also the type of influencing factors (e.g. social, economic, technical) may be different from the one validated for this case study. Therefore, it is recommended that a behavioral study is carried out allowing for validating the behavioral model, estimating the effect of the influencing factors, and measure the initial values of quantity and type of pesticide used.

Furthermore, the model has some potential for expansion and further development:

a) *Adapting to other pesticide application techniques and human behavior*: The model can be easily adapted to new application techniques. Thereby, the transfer-coefficients developed and applied for other pesticide models can be used as input values for the coefficients to the environmental compartments. For estimating the flow to the human compartment, however, experiments should be performed to estimating the amount of pesticides ending on human body. Similarly, the behavioral model will have to be adapted as the behavioral factors that were used in this case study may not explain pesticide application decisions in cases in which the application technique is not the knapsack sprayer. The theoretical framework used to inform the model in this case study [52] may be used to inform the study of pesticide application in different contexts, which will result in different behavioral equations, thus helping to adapt Be-Wetspa-Pest to other pesticide application techniques.

b) *Including pesticide uptake by plants through the root zone:* As a further development of the model a module on pesticide uptake into the crop through the root zone should be considered. This would allow to model a further channel of exposure to human health, namely through food consumption. Be-WetSpa-Pest models concentration of pesticide in the soil and therefore this can be used as input variable into a pesticide crop uptake model [69].

c) *Including different irrigation systems*: Some agricultural areas might have water reservoirs for agricultural purposes in addition to rain. The movement of the pesticides in soil might be affected in different ways depending on the irrigation techniques.

d) *Including second order degradation of the active ingredient*: One caveat of the model is that we considered for keeping the model easy manageable only the first order degradation of the active ingredient. We consider that given the high data uncertainties in developing countries, this is the right decision to take. If the model were adapted to regions with better data quality, it might be adequate to evaluate to which extent the inclusion of second order degradation of pesticides might make sense.

e) *Include horizontal redistribution in surface water*: In all compartments, except groundwater, the redistribution of pesticides, which is linked to water is vertically. This implies that horizontal distribution from plot to plot is not considered (and might be also very marginal). Future models could consider and complement the vertical redistribution with that horizontal redistribution.

f) *Modeling farmers´ behavior dynamically*: In Be-WetSpa-Pest, farmer decision making is modeled through a deterministic equation. This is partly due to the fact that it was not possible to quantify the influence of farmers' perception of e.g. pesticide infestation levels, or environmental quality on pesticide application decisions [53]. In fact, little evidence exist that farmers in Vereda La Hoya changed their pesticide application decisions because of the perception of environmental impact of pesticide use. However, in Be-WetSpa-Pest there is further scope for internalizing farmers' behaviour, i.e. to model not only the impact of pesticide application on the environment, but also how farmers respond to pesticide distribution and concentration in the environment should this be relevant for the study area to which the model is applied [53].

g) *Crop rotation:* There is an option in the model to implement crop rotation. This allows for accounting for different amounts of pesticide applied depending on the crops produced in the region.

h) *Modeling the effect of climate scenarios*: Be-WetSpa-pest presents no limitation to input meteorological data (rainfall, temperature, wind speed and direction) from downscaled climate scenarios. This application might be of relevance for the risk assessment analysis of climate impacts.

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Supporting information description.

Supporting information includes i) input variables and coefficients in WetSpa-Pest model, GIS layers derived from the DEM (Digital Elevation Model), simulated scenarios and funguicide application types (01 – Supporting information: Table 1, Table 2, Table 3, Table 4, Table 5), ii) detailed description of how pesticide application data and integration of farmer decision models into the WetSpa-Pest model are generated (02 - Supporting information: Generation pesticide application) and iii) detailed description and equations on the secondary distribution of pesticides in the modified PestLCI (03 - Supporting information: Redistribution and degradation processes of the pesticides).

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Tables captions

Table 1: Goodness of fit coefficients for the calibration and validation periods for water discharge.

Figures captions

Figure 1: Be-Westspa-Pest model structure including input, core model and output data.

Figure 2: Representation of the detailed software design of the integrative approach Be-WetSpa-Pest.

Figure 3: Comparison of measured (blue) and modeled (green) concentrations of Chlorpyrifos in soil (mg/kg soil) along the different growth stages of a potato field within the study region (La Hoya, Boyaca). Vertical bars denote standard deviation.

Figure 4: Simulation results for pesticide application of Mancozeb (six applications) on a sample field, for a total cycle of 140 days (method even). The triangles show the application dates. The dashed line and the continuous line show the soil respectively the topsoil concentration. The dotted line shows the concentration on the canopy.

Figure 5: Spatial distribution of Mancozeb concentration in the watershed. Four consecutives cycles were simulated (baseline scenario, method even). In the green marked areas no pesticides were applied during this simulation run.

Figure 6: Total amount of pesticide applied in one cycle (140 days) and the whole area. i: insecticide; f: fungicide

Figure 7: Spatial distribution of Mancozeb concentration in the watershed. Four consecutives cycles were simulated (8a: training scenario; 8b: cooperative scenario, method even). In the green marked areas no pesticides were applied during this simulation run.

Tables

Table 1:

Coefficient	Calibration	Validation
Model bias	-0.162	0.151
Nash-Sutcliffe efficiency	0.994	0.9966
RMSE	0.233	0.2375
Pearson coefficient	0.848	0.956
Standard error	0.012	0.008

Figures graphics

Figure 1:

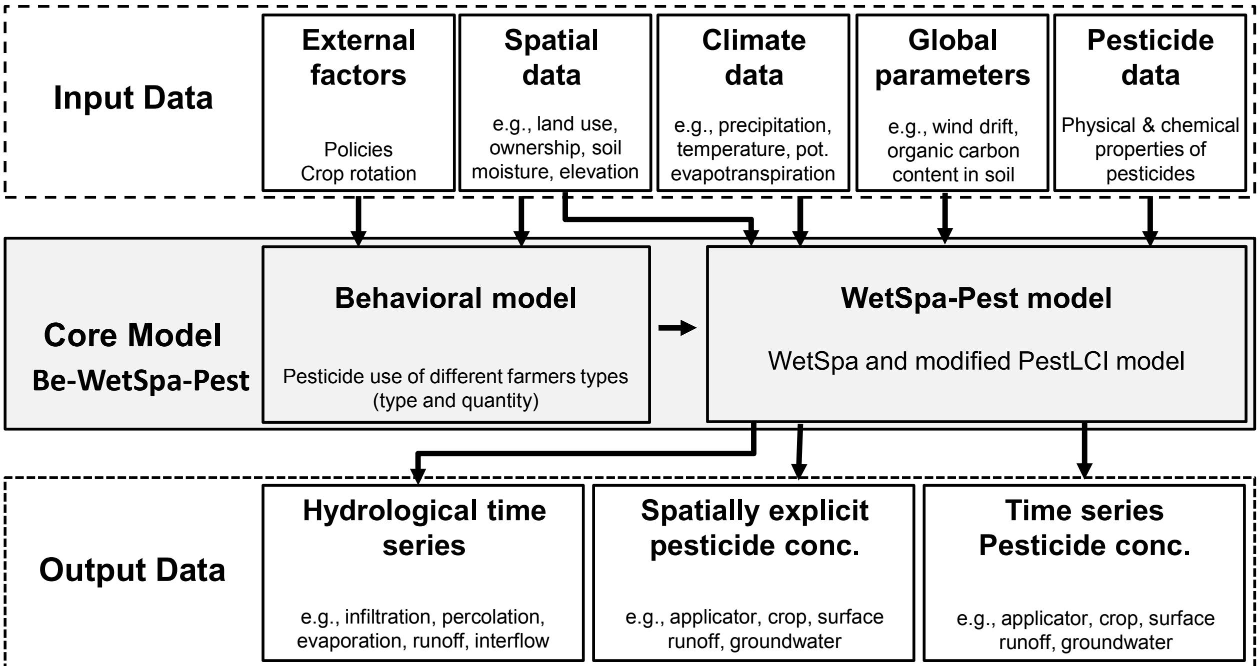
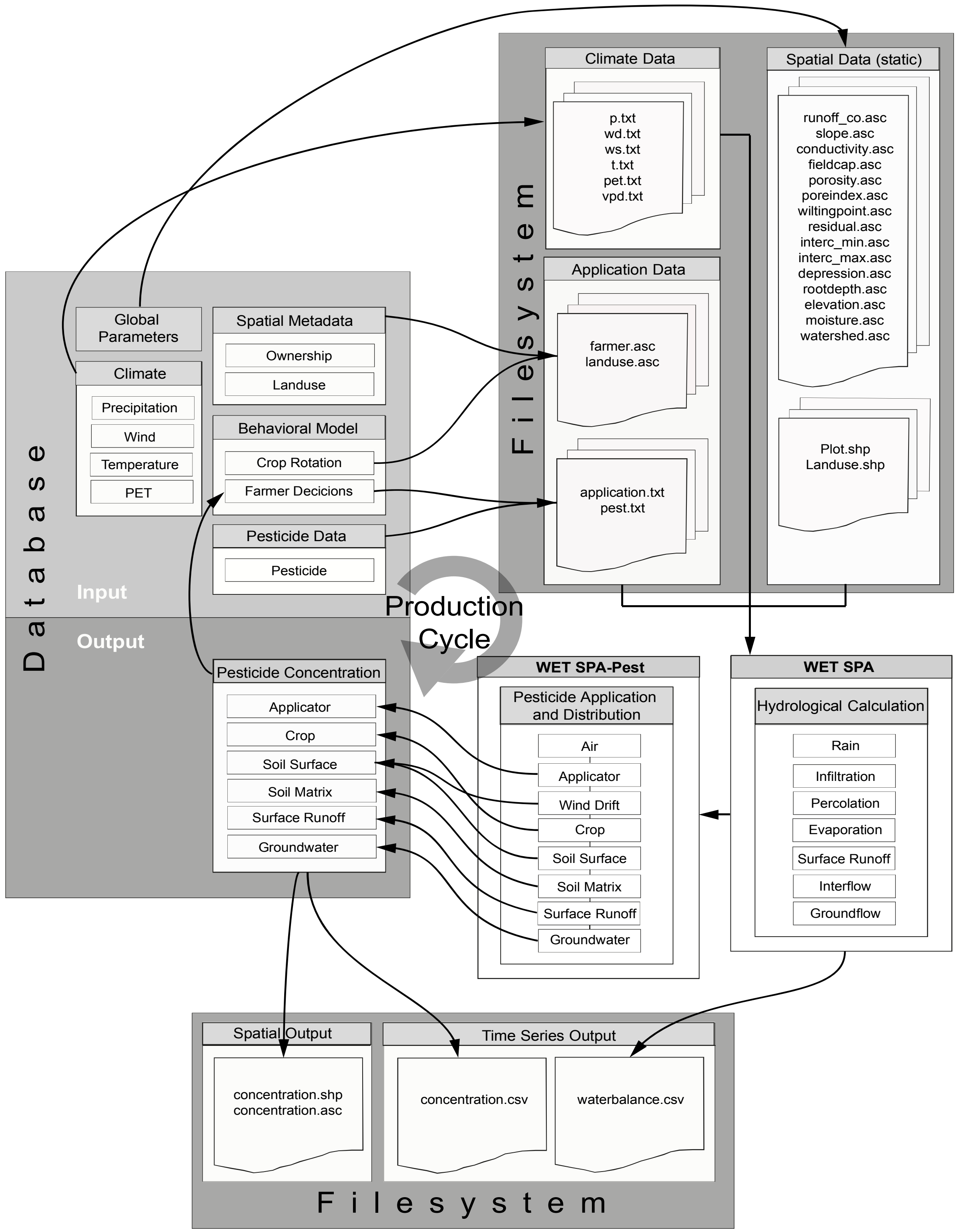


Figure 2:


Climate Data
p.txt
wd.txt
ws.txt
t.txt
pet.txt
vpd.txt
Spatial Data (static)
runoff_co.asc
slope.asc
conductivity.asc
fieldcap.asc
porosity.asc
poreindex.asc
wiltingpoint.asc
residual.asc
interc_min.asc
interc_max.asc
depression.asc
rootdepth.asc
elevation.asc
moisture.asc
watershed.asc
Application Data
farmer.asc
landuse.asc
application.txt
pest.txt
Plot.shp
Landuse.shp
Filesystem
Database
Global Parameters
Climate
Precipitation
Wind
Temperature
PET
Spatial Metadata
Ownership
Landuse
Behavioral Model
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Pesticide
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Crop
Soil Surface
Soil Matrix
Surface Runoff
Groundwater
WET SPA-Pest
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Surface Runoff
Groundwater
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Hydrological Calculation
Rain
Infiltration
Percolation
Evaporation
Surface Runoff
Interflow
Groundflow
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concentration.asc
Time Series Output
concentration.csv
waterbalance.csv
Filesystem

Figure 3:

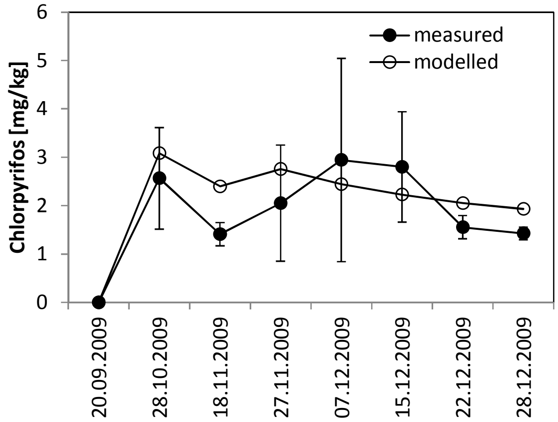


Figure 4:

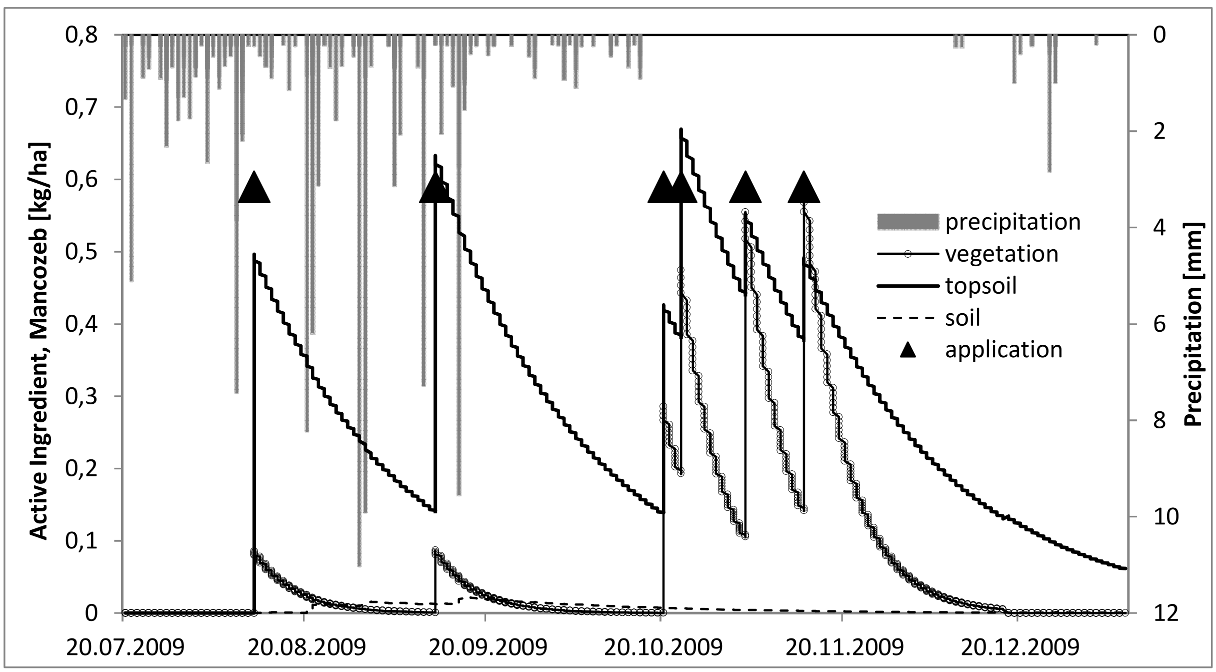


Figure 5:

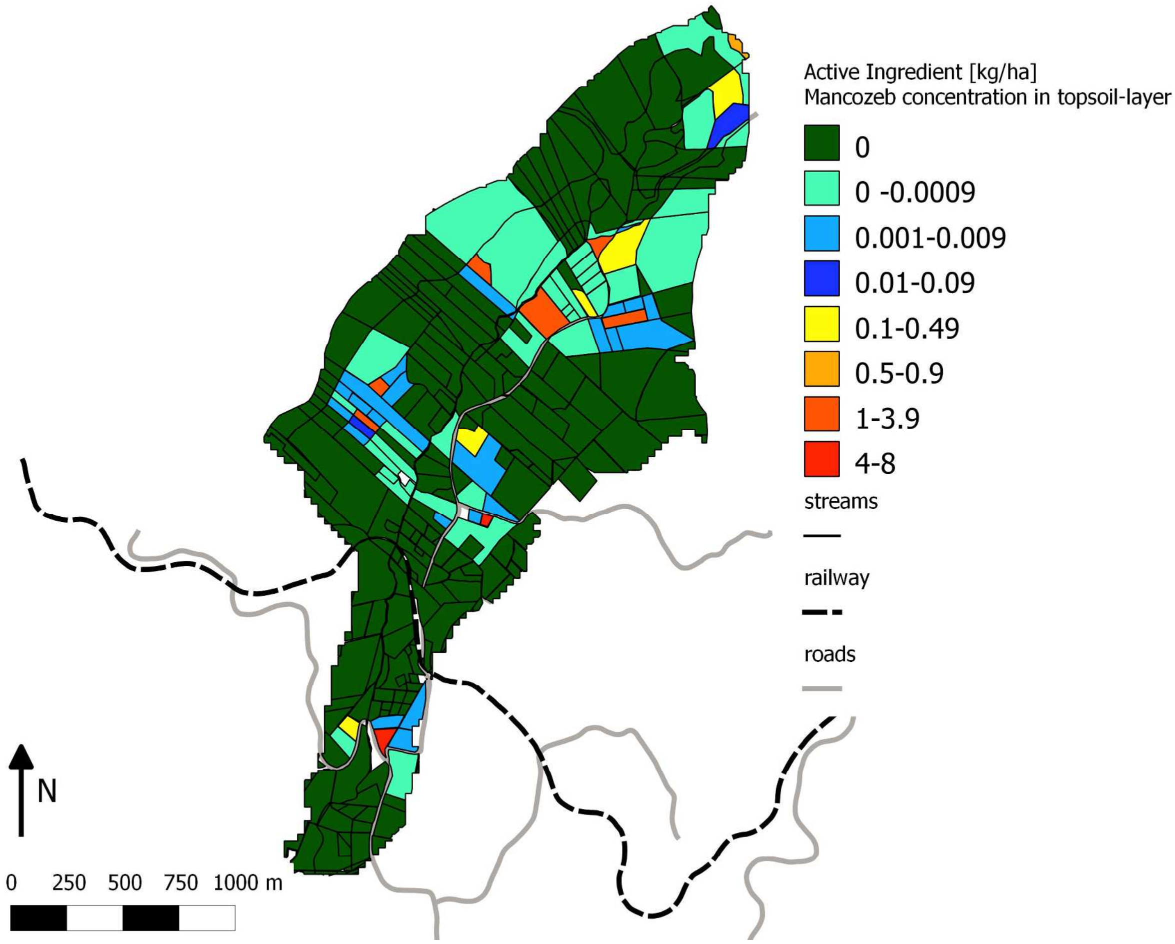

Active Ingredient [kg/ha]
Mancozeb concentration in topsoil-layer
0
0 -0.0009
0.001-0.009
0.01-0.09
0.1-0.49
0.5-0.9
1-3.9
4-8
streams
railway
roads
N
0 250 500 750 1000 m

Figure 6:

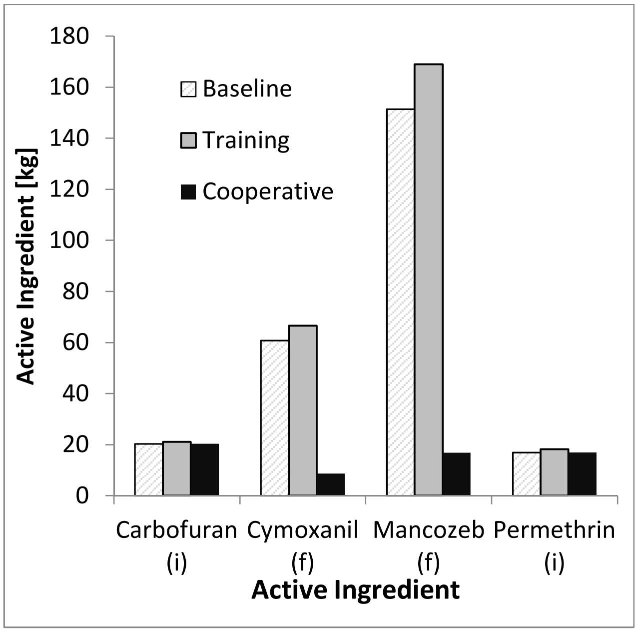
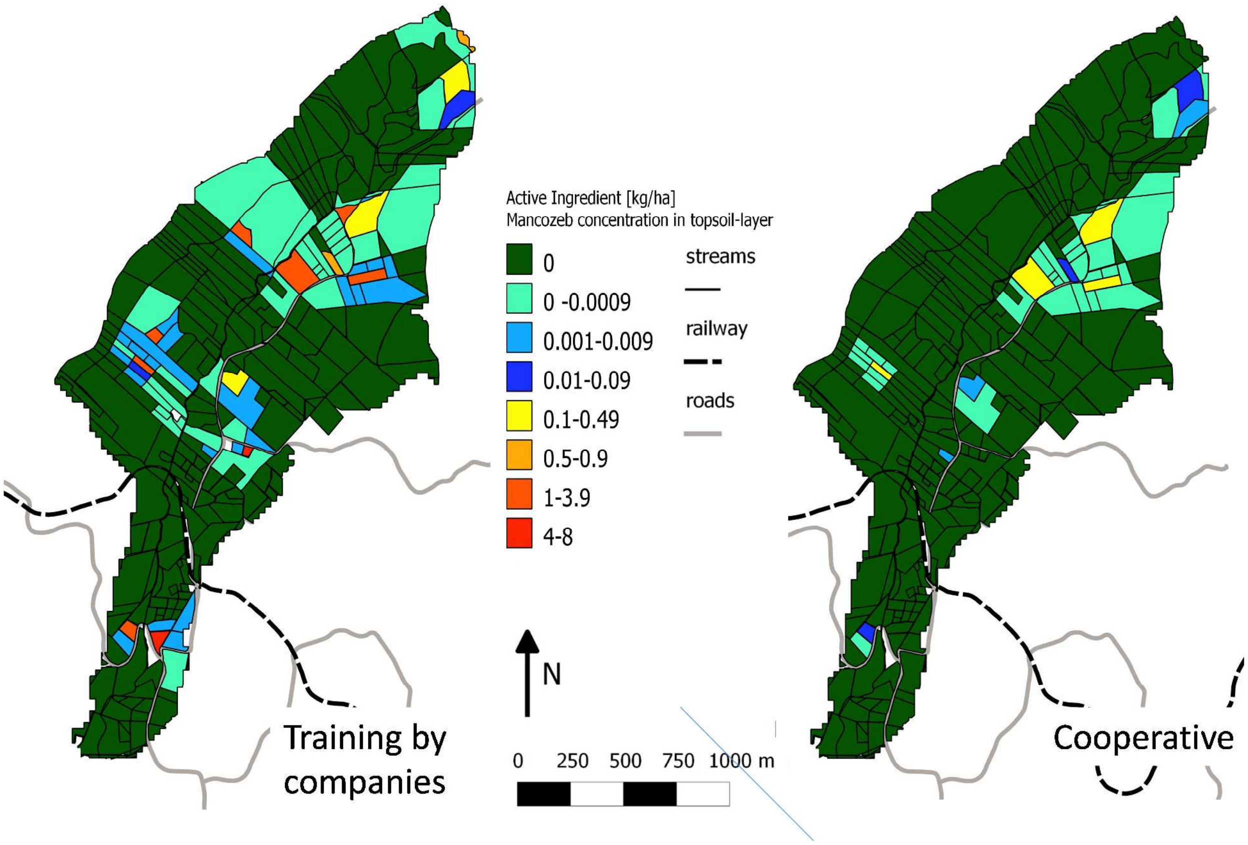
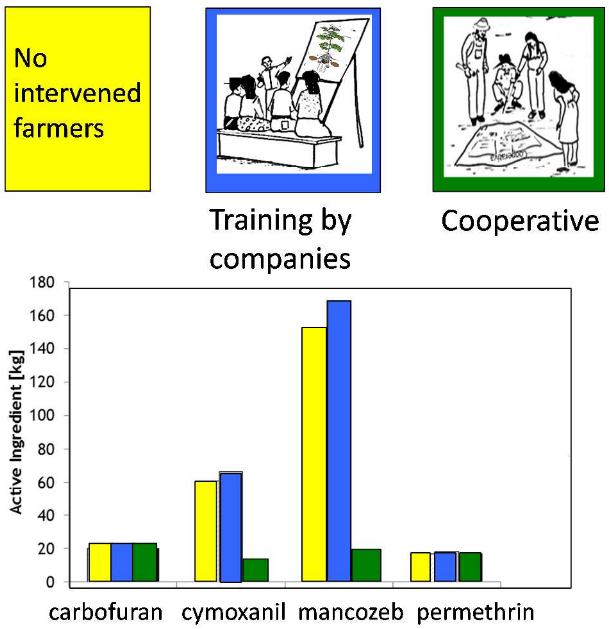

180
160
140
120
100
80
60
40
20
0
Active Ingredient [kg]
Baseline
Training
Cooperative
Carbofuran (i)
Cymoxanil (f)
Mancozeb (f)
Permethrin (i)
Active Ingredient

Figure 7:


Active Ingredient [kg/ha]
Mancozeb concentration in topsoil-layer
0
0 -0.0009
0.001-0.009
0.01-0.09
0.1-0.49
0.5-0.9
1-3.9
4-8
streams
railway
roads
N
0 250 500 750 1000 m
Training by companies
Cooperative

TOC graphic


No intervened farmers
Training by companies
Cooperative
Active Ingredient [kg]
0
20
40
60
80
100
120
140
160
180
carbofuran
cymoxanil
mancozeb
permethrin