



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

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

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13 **Abstract**

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

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

## 25 **Introduction**

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

32 Several tools have been developed to assess and reduce the impact of pesticides on the environment and  
33 on human health [9]. Of special interest in our case is the development and use of models. A first string  
34 of research develops environmental pesticide fate models. They analyze the distribution of pesticides  
35 within the environment, including plant, soil, water and in some cases through air (drift) (PEARL [10],  
36 CESMOS, BASINS (HSPF) ,[11]SWAT [12], Wet\_hydro [13], etc.). A particular group of models  
37 studies explicitly the contamination of water bodies. Models in this category are for example DRIPS,  
38 EXAMS, PIRANHA a/b/c (see [14] for a review). Other models, such as empirical curves, focus on  
39 pesticide airborne or drift deposition and were developed in the temperate region for terrestrial  
40 mechanized boom sprayers [15-19]. Some of these models perform optimally after calibration for the  
41 case of hand-held knapsack sprayers, mostly used in developing countries in the tropics, recently  
42 demonstrated by García-Santos et al. [20]. More sophisticated models focusing on pesticide exchange  
43 with the atmosphere after applied to soils and crops are dynamic and physically based [21]. The most  
44 advanced model within pesticide emission models is the PestLCI model [22,23] and was developed for  
45 use in agricultural life cycle assessment following mechanized spray application at local scale [24]. As

46 these models have all been developed for special needs and conditions of use, they differ in their spatial  
47 and temporal scales, time step, spatially explicitness, processes modeled, data requirements, complexity  
48 and output (see [14] for a review). Furthermore, most of these models have large data requirements and  
49 have never been applied in developing countries [25] and none of these models includes potential human  
50 exposure of the applicators as an output.

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

65 A third string of models combines agricultural production models (including pesticide use and to some  
66 extent environmental fate models) with economic models; an area where there has been significant  
67 progress in the last years (see [43] for a review; [44,45]). The integration of models ranges from linear  
68 programming models to spatially explicit multiple scales and multiple goal models [46,47]. A few

69 models analyze the effect of environmental degradation, e.g. erosion, water contamination on farmers'  
70 income and on the economic system at a regional level (e.g., ECECMOD [48]; and SAM [49]). The  
71 trade-off model [50] is the only integrative model that has been applied to pesticide management of  
72 potatoes in the Andes Region. It combines bio-physical models with econometric-process simulation  
73 models and provides an integrated analysis of tradeoffs between economic and environmental indicators.  
74 However, it has been found that farmers decision-making is often affected by parameters other than  
75 economic ones such as norms and traditions [51,52] and thus behavioral models are required which, on  
76 the one hand, simulate farmers' behavior and estimate the impacts of policies on pesticide use and, on  
77 the other hand, can be linked to spatially explicit pesticide models estimating the impact of behavioral  
78 change on human and environmental exposure. Finally, most models have high data requirements that  
79 cannot be met in developing countries and thus less data demanding models are required [40].

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

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

## 90 **Methods**

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

96 <Figure 1>

97 **Input data.** To run the model four types of data are needed (Fig. 1 and 2 in Database box; Table 1 in  
98 01\_Supporting information): “global parameters” as parameters required for the hydrological WetSpa  
99 model and pesticide emission PestLCI model, “climate data”, i.e., representative meteorological data of  
100 the catchment, “spatial metadata”, i.e., spatially explicit land use, catchment, weather station and  
101 appropriation data, “pesticide data”, i.e., physical and chemical properties of applied pesticides, and  
102 “external socio-economic factors”, i.e., policies and crop rotation. The input data are stored in form of  
103 different GIS layers (Fig.2 File system box; Table 3 in 01\_Supporting information). Ownership  
104 information was entered in GIS based on the latest Cadastral map [55]. Physical and chemical properties  
105 of applied pesticides within “pesticide data” were obtained from the PestLCI database and own  
106 empirical field experiments in similar soils [56,57].

107 <Figure 2>

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

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<sup>1</sup>Beta version available upon request.



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

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

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

150 The second part of Be-WetSpa-Pest model is the WetSpa-Pest model. WetSpa-Pest is a fully distributed,  
151 spatially explicit hydrology and emission pesticide model based on the WetSpa model by Liu and Smedt  
152 [54] and the here modified PestLCI model [22], respectively. The model WetSpa is a GIS-based  
153 distributed hydrological model for flood prediction and water balance simulation on a catchment scale  
154 (for more details on the water flows on a cell basis see [54]). It was developed by the Free University of  
155 Brussels and can be downloaded for free (<http://www.vub.ac.be/WetSpa/>). The pesticide emission model  
156 PestLCI was developed in Denmark by Birkved and Hauschild [22] (updated version in [23]) to provide  
157 information for the estimation of pesticide mass in the environment (air, surface water and groundwater)  
158 outside of the sprayed field after aircraft, boom spray (pull tractor) or soil injection application

159 techniques to be included in life cycle assessment. Its modular structure allows adaptation to conditions  
160 for different regions and agricultural practices and techniques. A human exposure component was added  
161 and drift fraction was modified for hand-held spray pest application (more details below).

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

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

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

$$181 \quad P_A = (P_V + P_D + P_H + P_L + P_S) P_A / 100 \quad (1)$$

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

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

189 Pesticide staying in the air ( $P_V$ ): The value for the pesticide staying in the air depends on the type of  
190 pesticide and meteorological conditions of the area. It can be entered into the model as a specific fixed  
191 value. In the case of Vereda La Hoya the value of 1 % was used given the measurements in the field  
192 [59].

193 Pesticide drifted by wind ( $P_D$ ): Hand-held spray is not a considered technique in the PestLCI or PestLCI  
194 2.0. For the case of hand-held spray in potato production, it is found that drift is higher as compared to  
195 conventional boom spray with tractor [61] and therefore the here modified PestLCI includes two  
196 possibilities a fix drift fraction of 3.1% of the applied dose as derived from García-Santos et al. [62] or  
197 calculation of drift for the first 20 m outside the plot in function of distance through the optimized  
198 IMAG drift calculator (v 1.1) by Holterman and Zande [16] (in PestLCI v2) after García-Santos et al.  
199 [61] (optimized parameters:  $a = 29$ ,  $b = -6.8$ ,  $c = 18.35$ ,  $d = -0.44$ ). Other equations in function of wind  
200 speed may reflect a more realistic scenario in cases where spray is conducted under wind conditions  
201 above  $2 \text{ m s}^{-1}$ , available in García-Santos et al. [61]. This could be added into the model structure.

202 Pesticide reaching the human ( $P_H$ ) (not in PestLCI 2.0):  $P_H$  is the fraction of the pesticide reaching the  
203 farmer's clothes and is calculated by using a fixed fraction of 1% of the total pesticide derived from  
204 empirical measurements [60]. The type of protection equipment used determines the final exposure of

205 the farmers [60]. In the case we applied the model, Vereda La Hoya, farmers use gummy boots, long  
206 trousers and a T-shirt covered by a “ruana” or “poncho”.

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

$$210 P_L = (P_A - P_H - P_D - P_V) * v_i \quad (3)$$

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

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

$$214 P_S = P_A - P_V - P_D - P_H - P_L \quad (4)$$

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

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

227 **Case study.** Be-WetSpa-Pest was implemented in a typical Andean mountainous region, the department  
228 (“Departamento”) of Boyacá, which contributes to ca. 26% of the national potato production and to 45%  
229 at regional level despite its low productivity, and its land tenants are mainly smallholders (95% of the  
230 workforce) [20, 70]. The same area of study has been focus of recent studies on human and  
231 environmental exposure from hand-held knapsack pesticide applications [20,39,40,44,45,  
232 52,53,60,61,62,64,69]. The study area Vereda La Hoya has 840 ha and is located in the district La Hoya  
233 of the community Tunja (Colombia) at a height of about 2800 to 3200 m a.s.l. It lies in the cold climate  
234 thermal floor zone, with a total mean annual rainfall of  $620 \pm 20$  mm. The area has prevailing south-east  
235 winds with average wind speed of  $1.8 \pm 1.39$  m s<sup>-1</sup> and a maximum of 7.6 m s<sup>-1</sup> (data from this study).  
236 Meteorological variables were registered every 15 min for 3 years, from October 2008 until October  
237 2011, at 3 m above ground, using a low cost automatic meteorological station, Davis Vantage Pro-2,  
238 installed within the watershed because no representative weather information was found in the national  
239 net (IDEAM).

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

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

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

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

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

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

274 <Table 1>

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

287 <Figure 3>

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



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

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

301 **The baseline scenario.** Figure 4 shows the simulation results for a specific plot of the active ingredient  
302 Mancozeb fungicide ( $C_8H_{12}MnN_4S_8Zn$ ), an ethylenebisdithiocarbamate (CAS Number:8018-01-7).  
303 On the top X-Axis and the right Y-Axis, precipitation on the plot is depicted, on the lower X-Axis and  
304 the left Y-Axis, the concentration of Mancozeb is shown. The first application (20.8.2009) took place at  
305 the start of the growth phase. The amount of Mancozeb intersected by the canopy is low, a large share of  
306 the Mancozeb applied (about 83 %) end in the topsoil and some infiltration occurs when there is  
307 precipitation. In the larger growth stage (20.10.2009), the plant intercepts a higher percentage of the  
308 pesticide leading to a lower amount reaching the topsoil (up to a share of about 48% for plant and  
309 topsoil). The amount infiltrating through the topsoil to the soil is rather below <4% and is favored is by  
310 precipitation due to the wash off from canopy to topsoil and from topsoil to soil. The total amount of  
311 Mancozeb accumulated in the soil is low and zero at the end of the cycle. On contrary, the concentration  
312 in the topsoil decreases slowly and one could potentially encounter residues even when the next cycle  
313 starts. This is not only due to the application itself, but also to the withering and degradation of the  
314 vegetation stubbles after harvesting the potatoes.

315 <Figure 4>

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

324 <Figure 5>

325 **Scenario analysis.** In the policy scenario ‘training by companies’ we simulate the effect of a training  
326 program held by pesticide producing companies. We considered only the farmers who had no  
327 intervention in the baseline scenario. For these farmers, the introduction of the policy modifies the  
328 probability of adopting one of three fungicide and insecticide application types respectively. This  
329 potentially determines a variation (i.e. increase) of pesticide released into the environment. The results  
330 show a marginal increase in productivity, but a significant increase in fungicide and insecticide use  
331 ([53]). In the policy scenario ‘cooperative’ we simulate the effect of the participation of farmers in  
332 producer cooperatives. The results show that this scenario significantly improves the efficacy of  
333 insecticide use, that is, it reduces insecticide use rates [53].

334 Figure 6 shows the total amount of active ingredient of two fungicides and two insecticides applied in  
335 the total area during one cycle (140 days) for the baseline and the two scenarios mentioned above.  
336 Regarding the insecticides, Carbofuran and Permethrin, almost no differences can be found between the  
337 scenarios, implying that these policy measures will not be effective in reducing exposure to pesticides in  
338 the case studied. For the fungicides Mancozeb and Cymoxanil the training by pesticide producing

339 companies significantly increases the amount of pesticides applied, whereas joining a cooperative  
340 reduces the amount of fungicides applied by almost 90%. This suggests that fostering cooperatives and  
341 providing training and production support through the cooperatives might be a good way forward to  
342 reduce the amount of fungicides applied. Even though this variable had a strong estimated effect on  
343 fungicide use it was not significant for insecticides use and was therefore not included in the equation.  
344 That is, insecticide and fungicide use are determined by different sets of factors, and even when there is  
345 one factor that influences both pesticide and insecticide use (e.g. the proportion of household income  
346 coming from agriculture), the coefficient is not the same in both equations for the two behaviors (as  
347 estimated in the statistical models [53]). This indicates the necessity for a disaggregated behavioral  
348 analysis for pesticide use rather than an overall analysis looking at the amount of money spent on  
349 pesticides.

350 <Figure 6>

351 When looking at the spatial distribution of Mancozeb (Figures 7 a,b), the amount of hotspots (>1 kg/ha)  
352 increases in the case of the training scenario, whereas the areas, where pesticide amounts higher than  
353 1kg/ha can be found in the topsoil is markedly reduced in the cooperative scenario. In particular, the  
354 concentration of Mancozeb in the areas close to the river is reduced. This result reflects the necessity of  
355 a spatially explicit analysis (see also [50]) to provide decision support for reducing surface water  
356 contamination by decreasing the pesticide concentration on plots close to surface water areas.

357 <Figure 7>

### 358 **Model use recommendations and further model developments.**

359 This paper presented Be-WetSpa-Pest, a simulation model that (i) integrates a hydrological model with  
360 an extended pesticide emission model considering environmental and human compartments; and (ii) is  
361 coupled to a behavioral model, for estimating the effect of different policies on farmers' pest control

362 behavior, affecting pesticide distribution in the environment and onto the applicator. The model was  
363 calibrated and validated for the case of Vereda La Hoya in Colombia and provided valuable results on  
364 the effect of policies on humans and environmental exposure to pesticides. We suggest the model to be  
365 applicable for similar cases in developing countries, where there is low data availability. However, we  
366 recommend, for the environmental part, to measure the key input variables for climate data like daily  
367 precipitation and temperature from a nearby station, and to obtain a DEM of the area to be studied for  
368 the spatial data.

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

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

380 a) *Adapting to other pesticide application techniques and human behavior*: The model can be easily  
381 adapted to new application techniques. Thereby, the transfer-coefficients developed and applied for  
382 other pesticide models can be used as input values for the coefficients to the environmental  
383 compartments. For estimating the flow to the human compartment, however, experiments should be  
384 performed to estimating the amount of pesticides ending on human body. Similarly, the behavioral

385 model will have to be adapted as the behavioral factors that were used in this case study may not  
386 explain pesticide application decisions in cases in which the application technique is not the  
387 knapsack sprayer. The theoretical framework used to inform the model in this case study [52] may  
388 be used to inform the study of pesticide application in different contexts, which will result in  
389 different behavioral equations, thus helping to adapt Be-Wetspa-Pest to other pesticide application  
390 techniques.

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

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

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

405 e) *Include horizontal redistribution in surface water:* In all compartments, except groundwater, the  
406 redistribution of pesticides, which is linked to water is vertically. This implies that horizontal

407 distribution from plot to plot is not considered (and might be also very marginal). Future models  
408 could consider and complement the vertical redistribution with that horizontal redistribution.

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

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

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

423

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430

431 **Supporting information description.**

432 Supporting information includes i) input variables and coefficients in WetSpa-Pest model, GIS layers  
433 derived from the DEM (Digital Elevation Model), simulated scenarios and fungicide application types  
434 (01 – Supporting information: Table 1, Table 2, Table 3, Table 4, Table 5), ii) detailed description of  
435 how pesticide application data and integration of farmer decision models into the WetSpa-Pest model  
436 are generated (02 - Supporting information: Generation pesticide application) and iii) detailed  
437 description and equations on the secondary distribution of pesticides in the modified PestLCI (03 -  
438 Supporting information: Redistribution and degradation processes of the pesticides).

439

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627 **Tables captions**

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

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### 630 **Figures captions**

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

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

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

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

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

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

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

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### 649 **Tables**

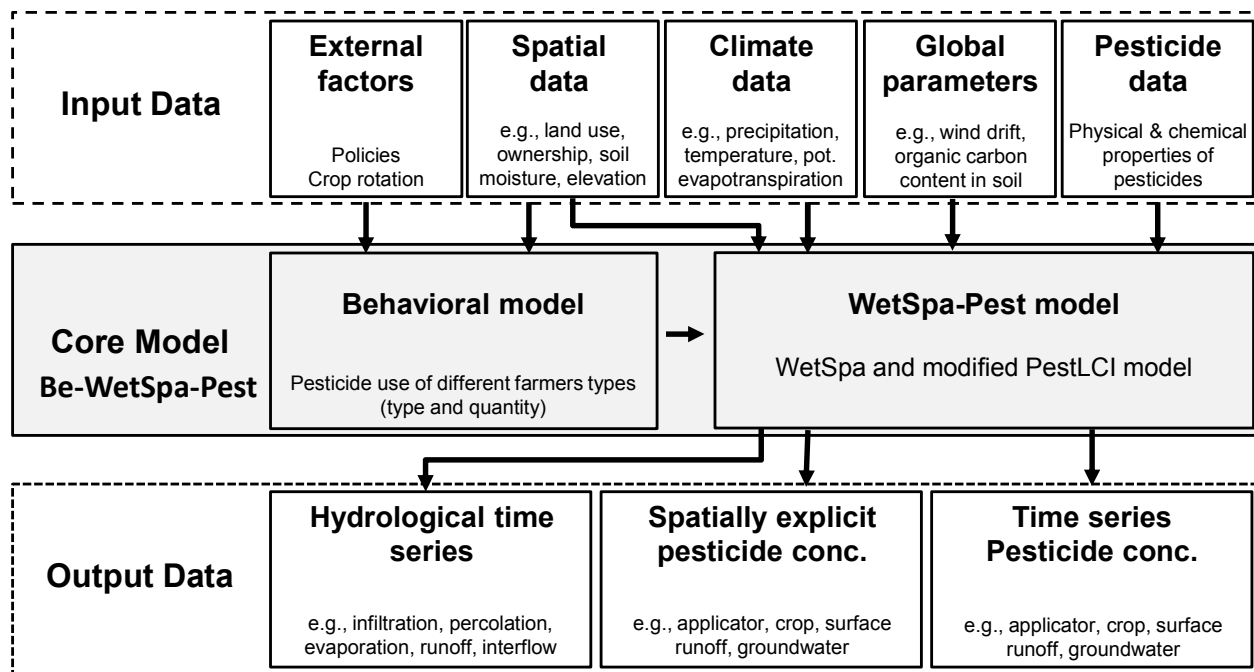
650 **Table 1:**



| 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      |

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653 **Figures graphics**654 **Figure 1:**

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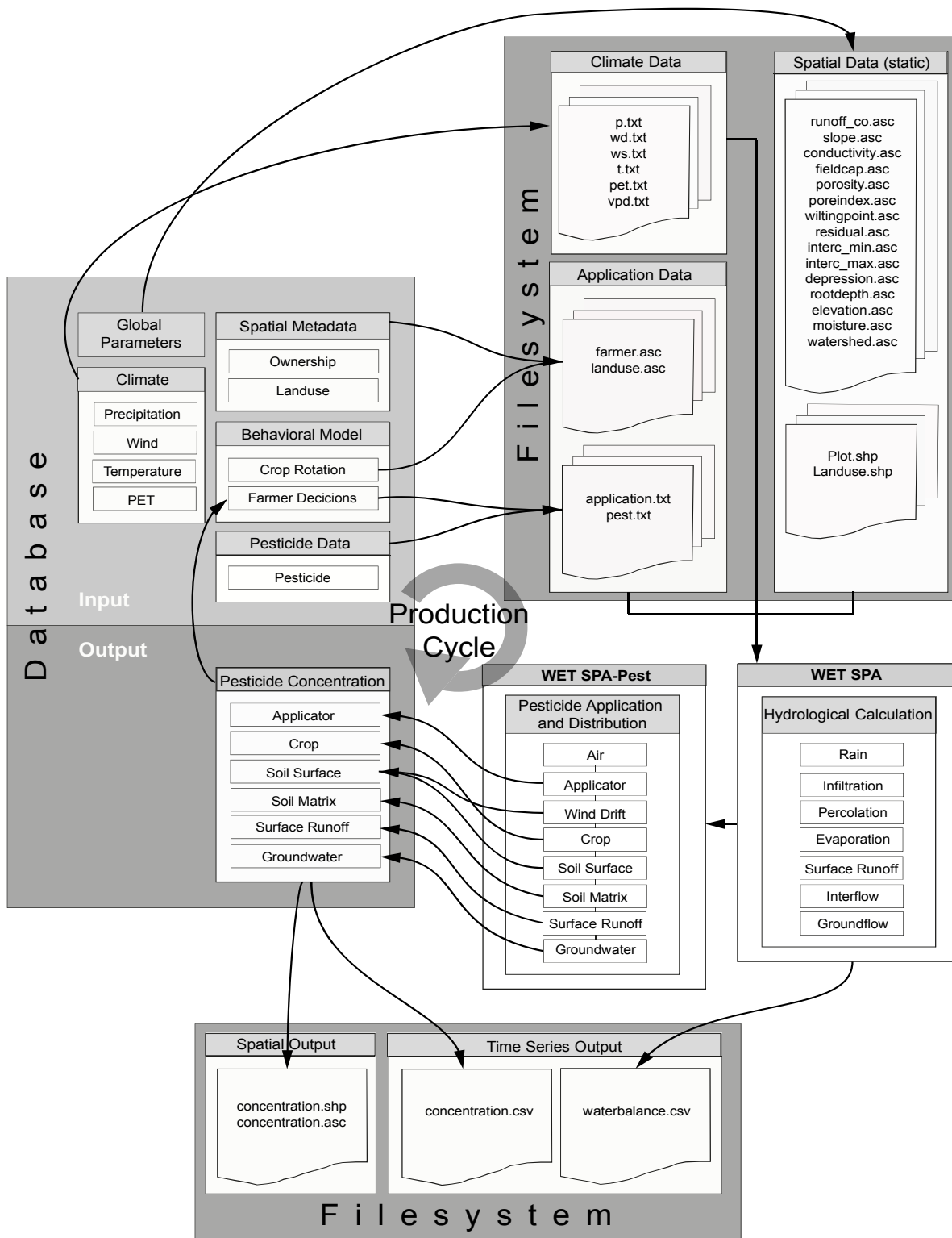
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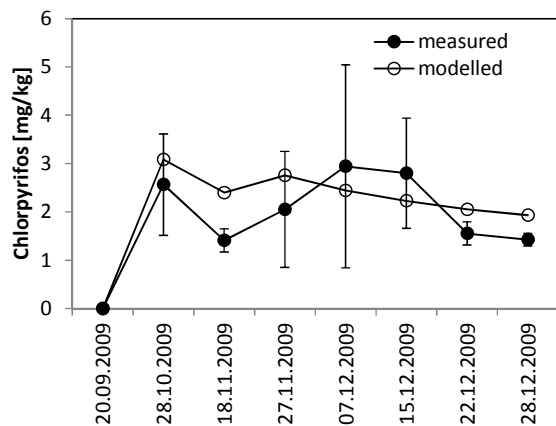
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667 **Figure 2:**

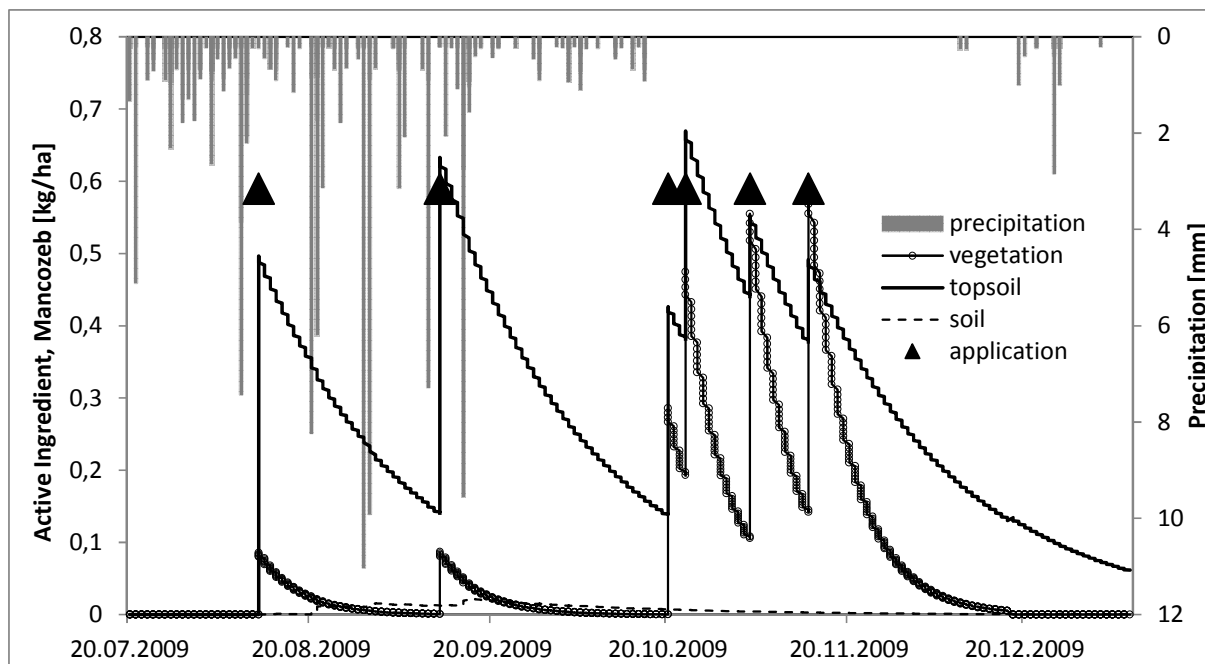


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670 **Figure 3:**

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672 **Figure 4:**

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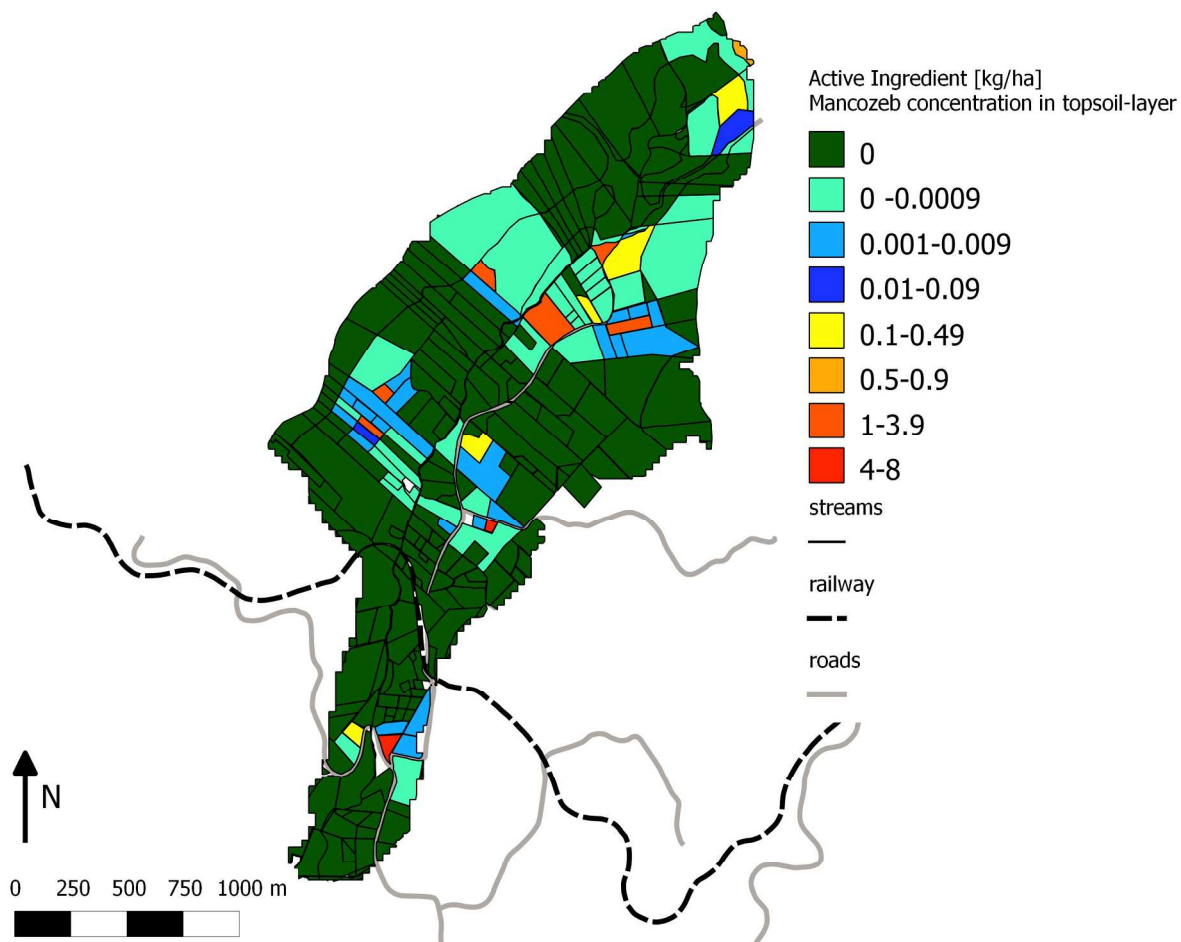
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680 **Figure 5:**

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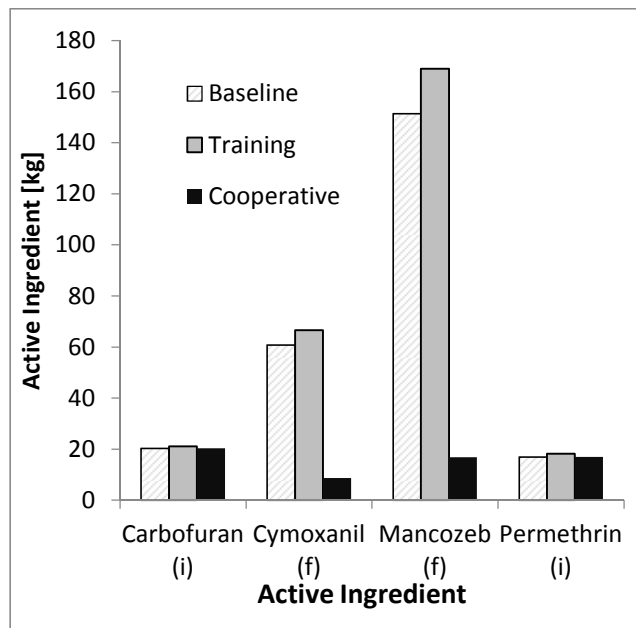
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691 **Figure 6:**

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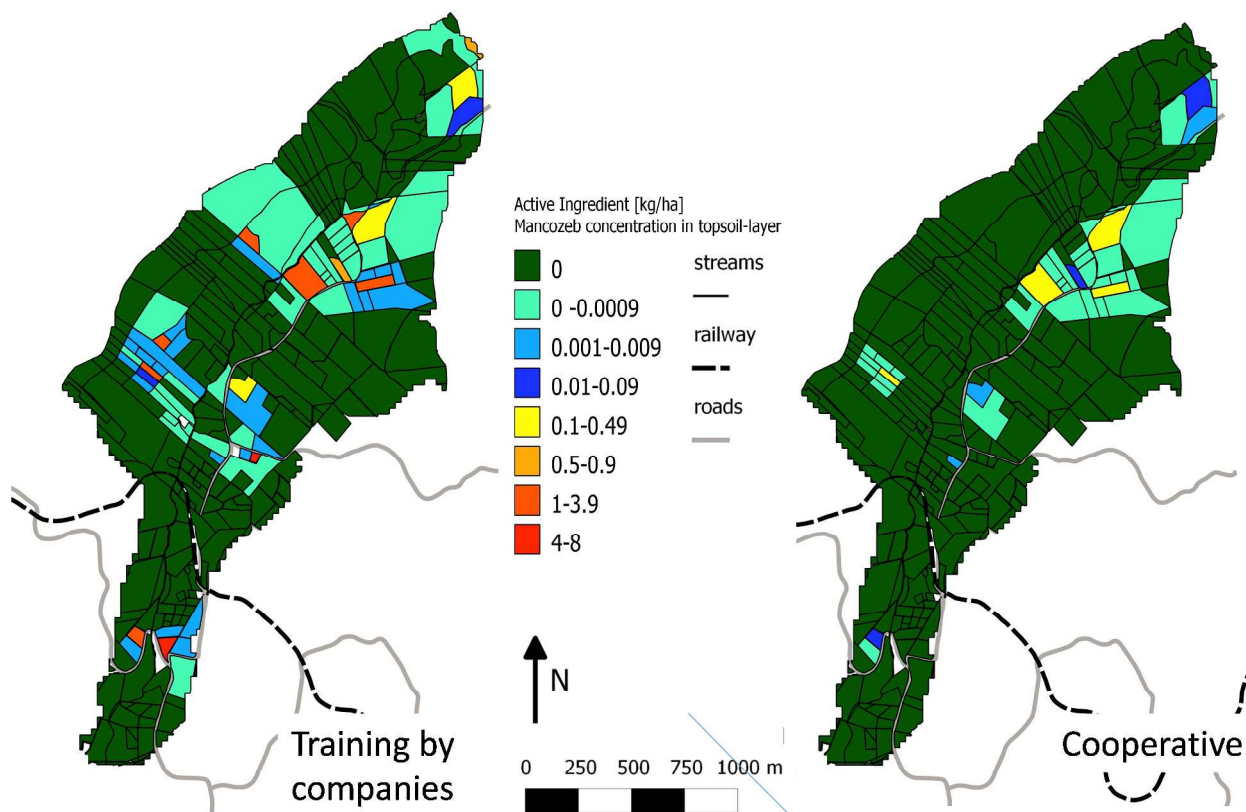
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707 **Figure 7:**



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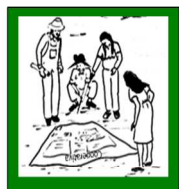
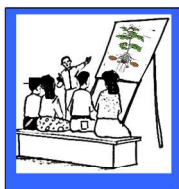
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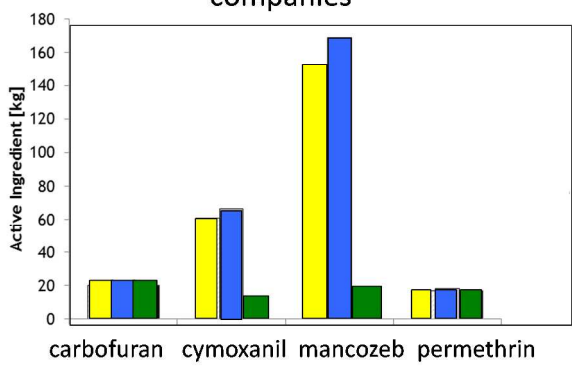
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719 TOC graphic



Training by companies

Cooperative



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