The effect of crop rotation on pesticide leaching in a regional pesticide risk assessment

Matteo Balderacchi, Andrea Di Guardo, Costantino Vischetti, Marco Trevisan

Supporting Information

Summary

been ranked into 4 leaching classes and the relative distribution percentages are shown. The difference in the class size between the lognormal and the normal distribution function is reported.

Figure S1. Comparison of the crop rotation winter cereal - maize modelled using MACRO 5.0 and FitoMarche without and with "bare soil crop". Yellow and green areas represent the target vegetative periods for maize and wheat, and dots represent the generated data. The plots on the left show the daily canopy evaporation (CETC) and those on the right, the pesticide concentration in micropores (SOILMIC 3-5 cm).

Figure S2. Climates of the Region Marche as reported in the climatic map from ASSAM

Figure S3. Thickness of profiles reported in the soil map of the Marche region (1:250000)

Figure S4. Dispersion chart showing the relationship between soil profile depth and organic carbon content in the topsoil.

Figure S5. Top layer Organic Carbon content reported in the soil map of the Marche region (1:250000)

Figure S6. Pesticide leaching maps for herbicide "A" results from tier 1 (S6a) and 2 (S6b); pesticide leaching maps for herbicide "B" results from tier 1 (S6c) and 2 (S6d);

Additional text. Main Concepts About FitoMarche

Table S1. Macro input values used to test the crop rotation.

Group	MACRO parameter	Maize parameter value	Wheat parameter value	Bare crop parameter value
CROP	ROOTINIT	1.00E-02	2.00E-01	
	ROOTMAX	1.00E+00	6.00E-01	
	CFORM	1.70E+00	2.00E+00	1e-19
	RPIN	6.70E+01	6.00E+01	
	CRITAIR	5.00E+00	5.00E+00	
	BETA	2.00E-01	1.00E-01	
	CANCAP	3.00E+00	3.00E+00	
	ZALP	1.00E+00	1.00E+00	
	IDSTART	95	288	365
	IDMAX	195	75	365
	IHARV	260	150	365
	ZHMIN	1.00E-02	2.00E-01	
	LAIMIN	1.00E-02	1.00E+00	1e-19
	LAIMAX	5	6	1e-19

	ZDATEMIN	96	65	365
	DFORM	3.00E-01	2.00E-01	1e-19
	LAIHAR	2.00E+00	2.00E+00	
	HMAX	1.80E+00	8.00E-01	
	ATTEN	6.00E-01	5.00E+01	
IRRIGATION	AMIR	3.00E+00	3.00E+00	
	CONCI	4.33E+01	2.33E+01	
	IRRDAY	9.10E+01	2.77E+02	
	NIRR	1.00E+00	1.00E+00	

ROOTINIT Root depth at the date ZDATEMIN [m]; ROOTMAX: Maximum root depth [m]; CFORM: Form factor for the period from emergence to maturity [-]; RPIN: Percentage of the root length in the top 25 % of the root depth. [%]; CRITAIR: Critical soil air content for water uptake [%]; BETA: Root adaptability factor [-]; CANCAP: Canopy interception capacity [mm]; ZALP: Correction factor for evaporation from wet canopy [-]; IDSTART: Day of crop emergence [d (giulian)]; IDMAX: Day of maximum leaf area / root depth [d (giulian)]; IHARV: Day of harvest [d (giulian)]; ZHMIN: Crop height at the date ZDATEMIN [m]; LAIMIN: The LAI at the date ZDATEMIN [-]; LAIMAX: LAI at maturity [-]; ZDATEMIN: this is used to define an intermediate crop development stage between emegence and maximum leaf ares. [d (giulian)]; DFORM: Form factor for the period from maturity to harvest [-]; LAIHAR: LAI at harvest [-]; HMAX: Maximum crop height [m]; ATTEN: Attenuation factor for solar radiation in a crop canopy [-]; AMIR: Amount of irrigation [mm]; CONCI:

solute concentration [g m-3]; IRRDAY: day of application [d (giulian)]; NIRR: number of applications [-]

Table S2. Temporal sequence used to model crop rotation.

Event	Change of parameters for crop development	Change of parameters for crop irrigation
Start	Crop1	Crop1
Day after the harvesting of the crop1	Bare soil	Crop2
day before the emergence of crop 2	Crop2	(no changes)
Day after the harvesting of the crop 2	Bare soil	Crop3
day before the emergence of crop 3	Crop3	(no changes)
Day after the harvesting of the crop 3	Bare soil	Crop4
Etc…		

Table S3. Crop rotations used in the simulation

Crop rotation number	Sequence
1	maize, winter cereal, sugarbeet, winter cereal
2	maize, winter cereal, fodder, fodder
3	maize, winter cereal
4	maize, winter cereal, fodder
5	maize, winter cereal, sunflower, winter cereal
6	maize, winter cereal, sunflower, winter cereal, fodder
7	sugarbeet, winter cereal, winter cereal
8	sugarbeet, winter cereal, sunflower, winter cereal
9	sugarbeet, winter cereal, sunflower, winter cereal, sunflower
10	sugarbeet, winter cereal, winter cereal, sunflower, winter cereal
11	sugarbeet, winter cereal, fodder, winter cereal
12	sugarbeet, winter cereal, sunflower, winter cereal, fodder
13	sugarbeet, winter cereal, fodder, winter cereal, fodder

14	sugarbeet, winter cereal, fodder, winter cereal, winter cereal
15	sunflower, winter cereal, fodder, winter cereal
16	sunflower, winter cereal, sunflower, winter cereal, fodder
17	winter cereal, winter cereal, sunflower
18	fodder, sunflower, winter cereal
19	winter cereal, sunflower, fodder, fodder
20	winter cereal, sunflower, winter cereal, sunflower, winter cereal, fodder
21	winter cereal, sunflower, winter cereal, fodder, fodder
22	sunflower, winter cereal, winter cereal, winter cereal, fodder
23	sunflower, winter cereal, winter cereal, winter cereal, fodder, fodder
24	fodder
25	fodder, fodder, fodder, winter cereal
26	winter cereal, fodder, fodder
27	fodder, winter cereal
28	vegetables, winter cereal, vegetables, winter cereal, vegetables, winter cereal, fodder
29	vegetables, winter cereal, winter cereal, winter cereal, fodder

30	fodder, fodder, fodder, fodder, beans
31	vegetables, winter cereal, winter cereal, sugarbeet, sunflower

Table S4. Temperature, precipitation and Potential Evapo-Transpiration of the region Marche climates

	Temperature [°C]	Precipitation [mm]	PET [mm]
Adriatic	13.7	687	742
Middle belt	13.5	693	697
Inland	11.5	715	776

Table S5. Properties and application schemes of the agrochemicals studied

Compound	Crop	Crop emergence (IDSTART)	Application day (IRRIDAY)	Application rate [g ha^{-1}]
Herbicide “A”	Maize	100	95	844
Herbicide “B”	Maize	100	95	1440
Herbicide “B”	Sugar beet	82	76	480
Herbicide “B”	Sunflower	61	51	1200
Insecticide “A”	Maize	100	182	3
Herbicide “C”	Winter cereal	288	283	909

Herbicide “D”	Winter cereal	288	283	97
Herbicide “E”	Sugar beet	82	87, 97	1200 x 2 appln
Herbicide “F”	Sugar beet	82	87, 97	60 x 2 appln
Fungicide “A”	Sugar beet	82	187, 208	100 x 2 appln

Table S6. KOC, ADI, DT50, and maximum mean annual concentration in leachate of the assessed compounds

	KOC	DT50	ADI	Maximum mean annual concentration in leachate recorded in the assessment [μg l^{-1}]
Fungicide “A”	1039	61	0.004	2.45
Herbicide “A”	220	88	0.003	35.77
Herbicide “B”	226	15	0.08	35.93
Herbicide “C”	8750	181	0.02	3.78
Herbicide “D”	601	105	0.5	3.48
Herbicide “E”	81	12	0.011	54.21
Herbicide “F”	130	15	0.13	2.19
Insecticide “A”	460000	26	0.01	0.00

Table S7. Acceptance or rejection tests of the distribution function fitting for Herbicides “A” and “B”. The table reports the percentage of cases that were not rejected by the tests.

Universe cluser	test	distribution function			
		Exponential	Gamma	Lognorm	Normal
herbicide "A" tier3	A-D test	10%	20%	60%	0%
herbicide "B" tier3	A-D test	0%	0%	60%	0%
herbicide "A" tier3	K-S test	0%	10%	60%	0%
herbicide "B" tier3	K-S test	0%	0%	60%	0%

Table S8. Effect of the data distribution function on leaching using the 80th percentile of the mean annual concentration and considering two distribution functions. The simulated regional areas have been ranked into 4 leaching classes and the relative distribution percentages are shown. The difference in the class size between the lognormal and the normal distribution function is reported.

Herbicide "A"									
	Step1			Step2			Step3		
	LogNor	Norm	LogNor - norm	LogNor	Norm	LogNor - norm	LogNor	Norm	LogNor - norm
0-0.1	0.1%	0.1%	0.0%	1.0%	1.0%	0.0%	6.8%	6.8%	0.0%
0.1-1	2.4%	2.4%	0.0%	12.7%	12.7%	0.0%	8.1%	8.1%	0.0%
1-10	27.4%	26.7%	0.7%	36.0%	36.2%	-0.2%	82.9%	64.9%	18.1%
>10	70.1%	70.8%	-0.7%	50.2%	50.1%	0.2%	2.1%	20.2%	-18.1%

Hebicide "B"									
	Step1			Step2			Step3		

	LogNor	Norm	LogNor - norm	LogNor	Norm	LogNor - norm	LogNor	Norm	LogNor - norm
0-0.1	18.1%	17.2%	0.9%	8.6%	8.7%	-0.1%	16.0%	49.6%	-33.6%
0.1-1	19.3%	10.2%	9.1%	34.7%	33.6%	1.2%	48.5%	27.1%	21.4%
1-10	39.4%	41.7%	-2.4%	47.0%	45.9%	1.1%	35.5%	20.5%	14.9%
>10	23.3%	30.9%	-7.6%	9.7%	11.9%	-2.2%	0.0%	2.7%	-2.7%

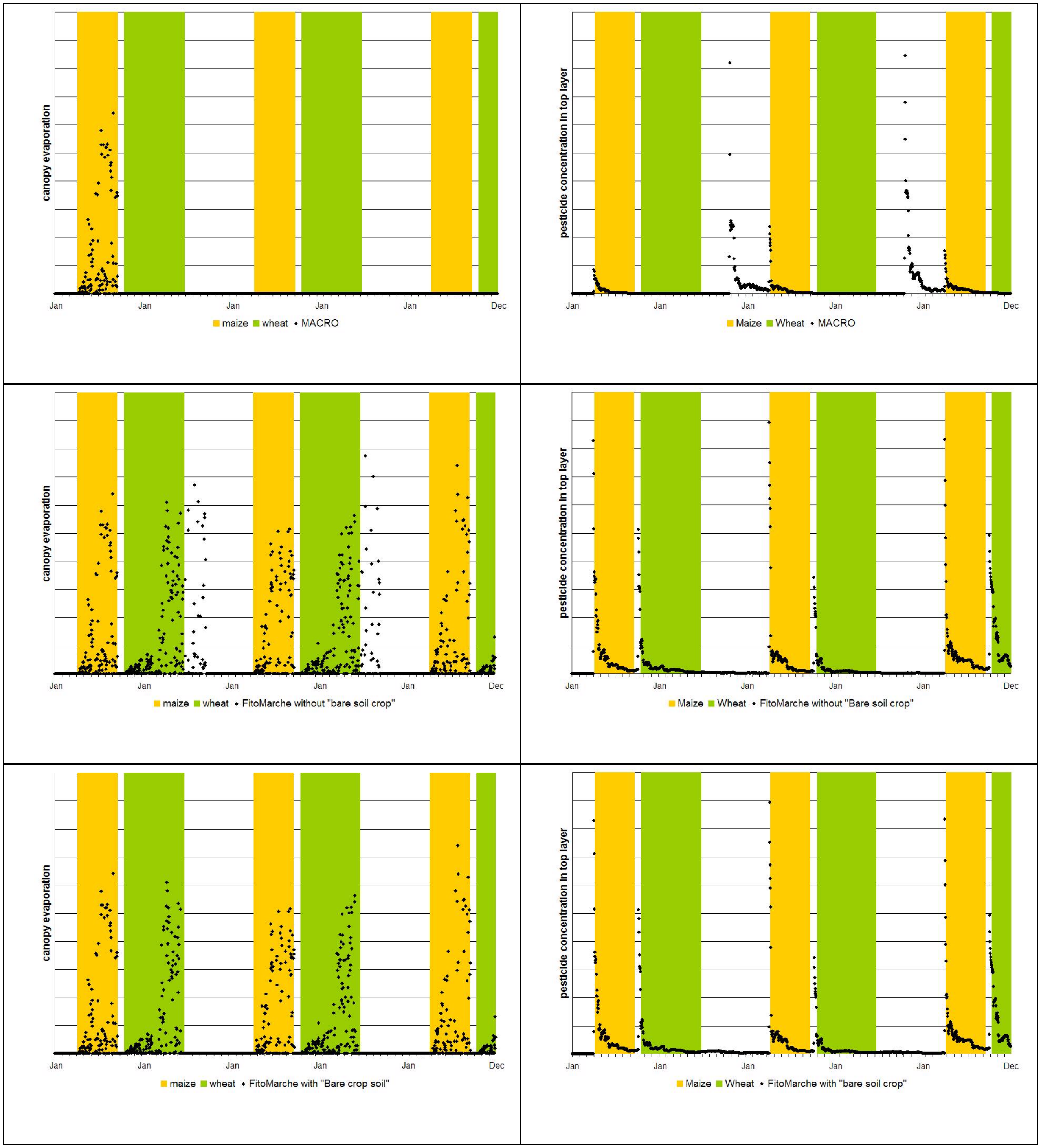


Figure S1. Comparison of the crop rotation winter cereal - maize modelled using MACRO 5.0 and FitoMarche without and with “bare soil crop”. Yellow and green areas represent the target vegetative periods for maize and wheat, and dots represent the generated data. The plots on the left show the daily canopy evaporation (CETC) and those on the right, the pesticide concentration in micropores (SOILMIC 3-5 cm).

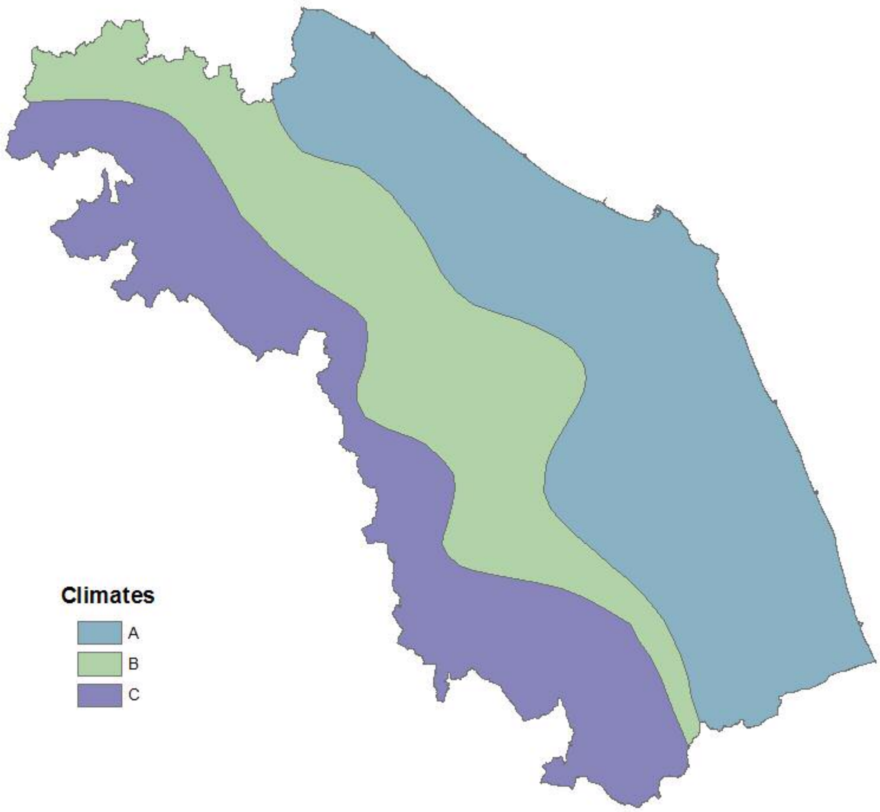


Figure S2. Climates of the Region Marche as reported in the climatic map from ASSAM

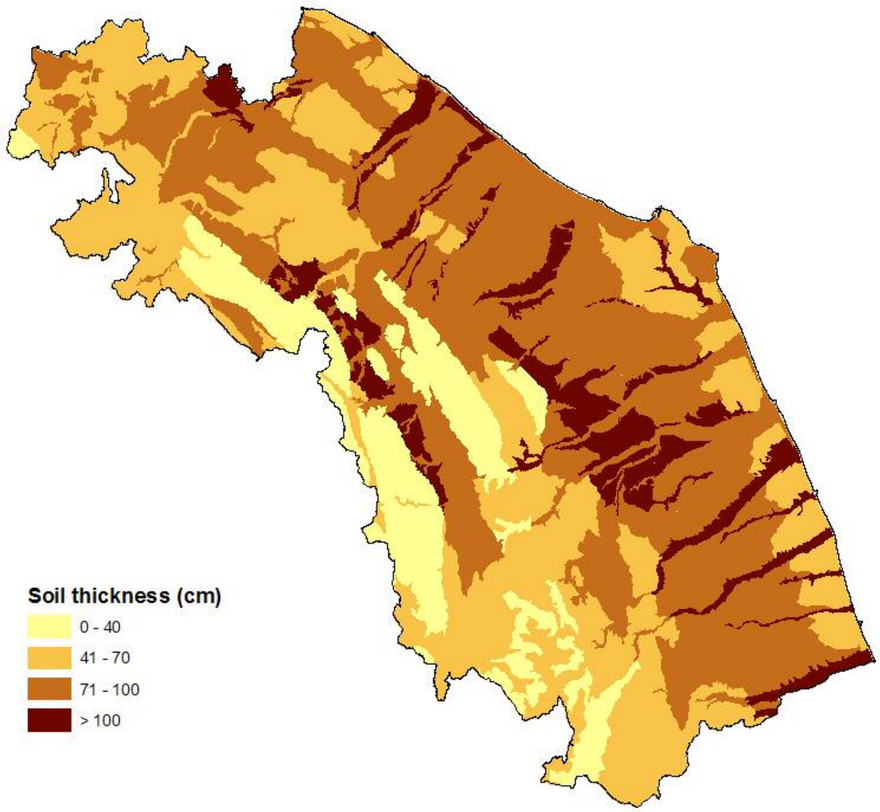


Figure S3. Thickness of profiles reported in the soil map of the Marche region (1:250000)

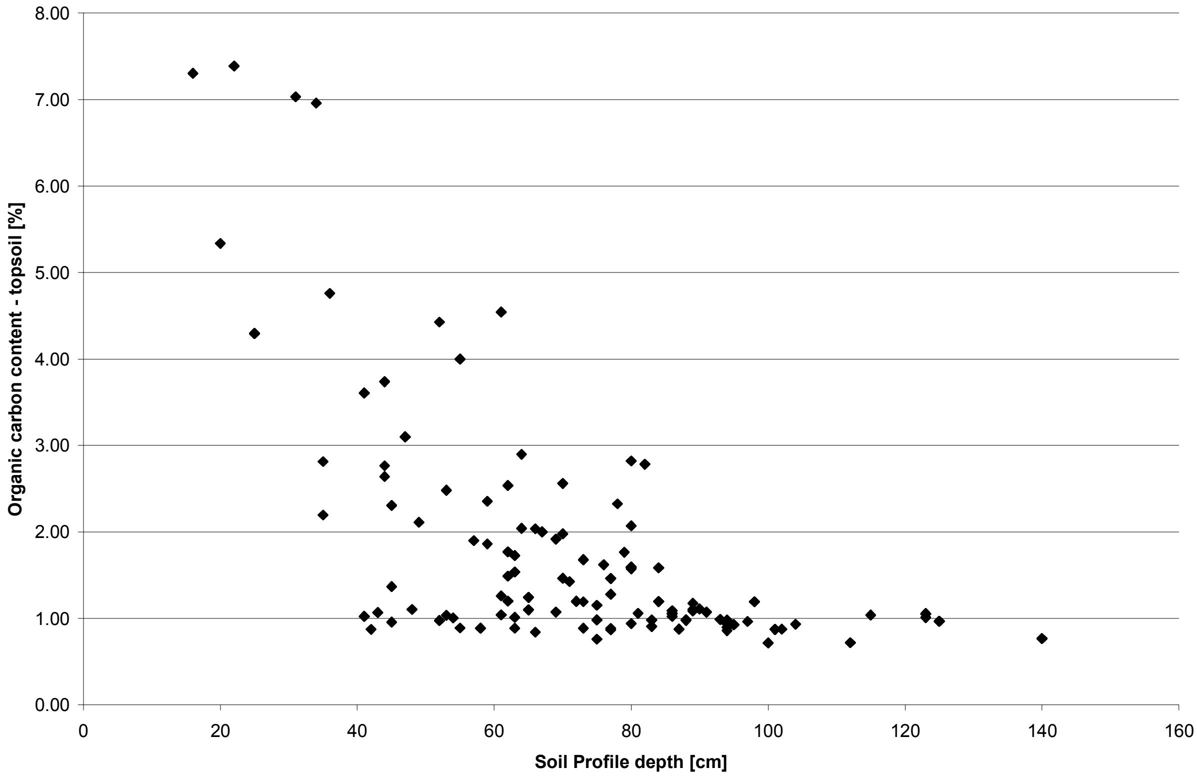


Figure S4. Dispersion chart showing the relationship between soil profile depth and organic carbon content in the topsoil.

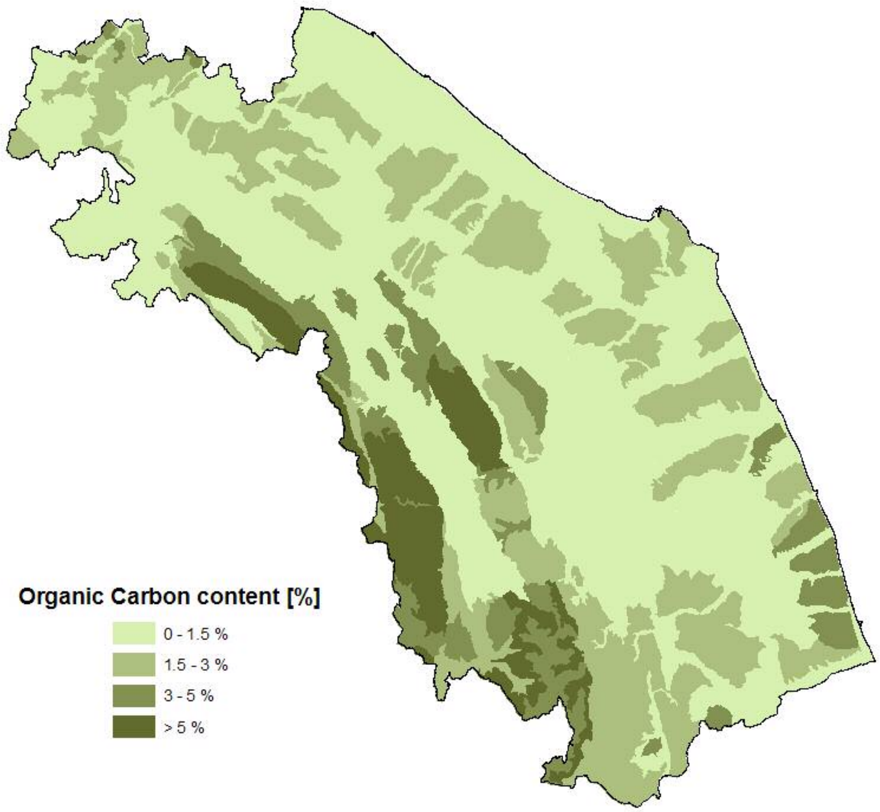


Figure S5. Top layer Organic Carbon content reported in the soil map of the Marche region (1:250000)

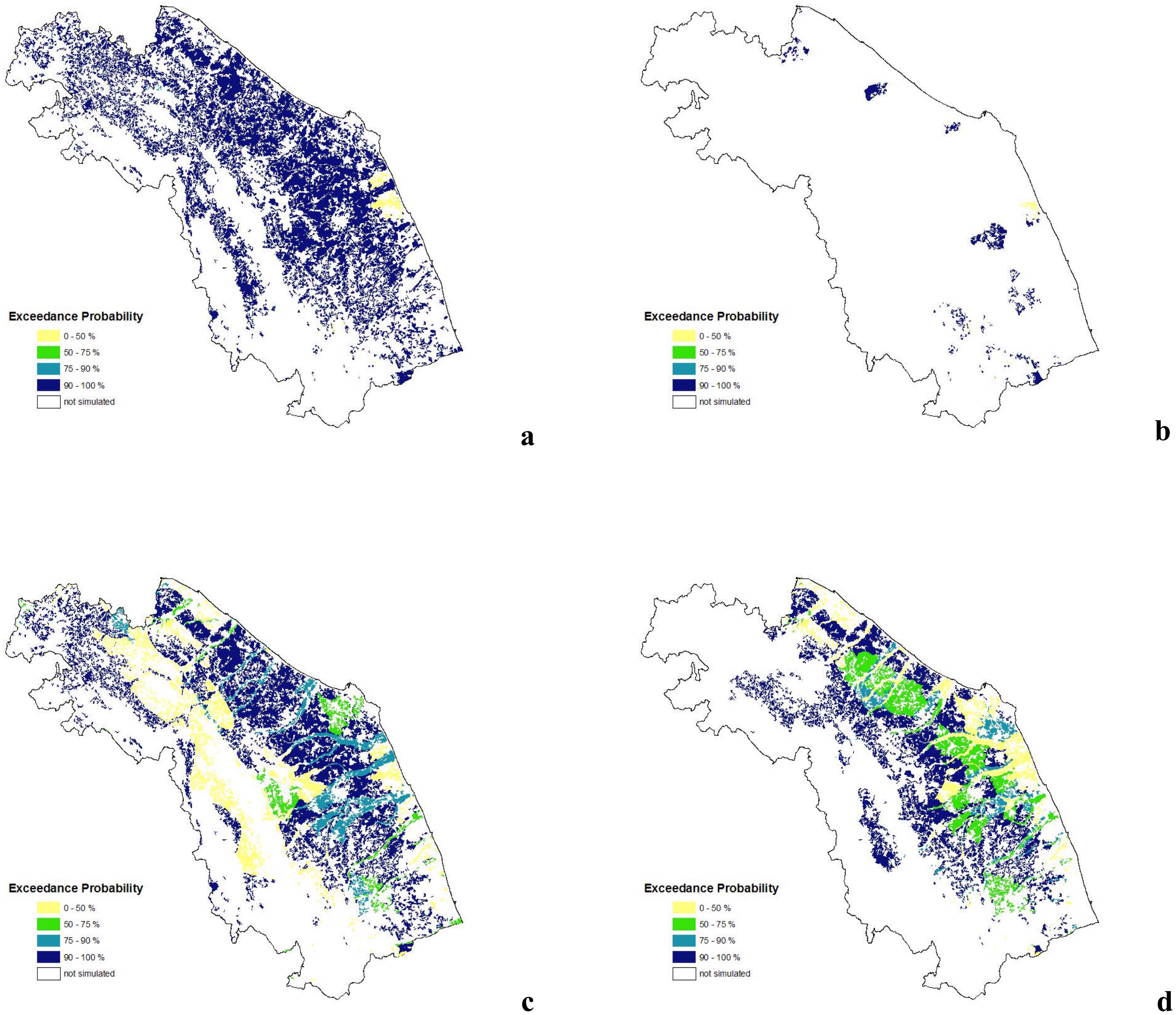


Figure S6. Pesticide leaching maps for herbicide “A” results from tier 1 (S6a) and 2 (S6b); pesticide leaching maps for herbicide “B” results from tier 1 (S6c) and 2 (S6d);

MAIN CONCEPTS ABOUT FITOMARCHE

What are the intended uses and users of the program?

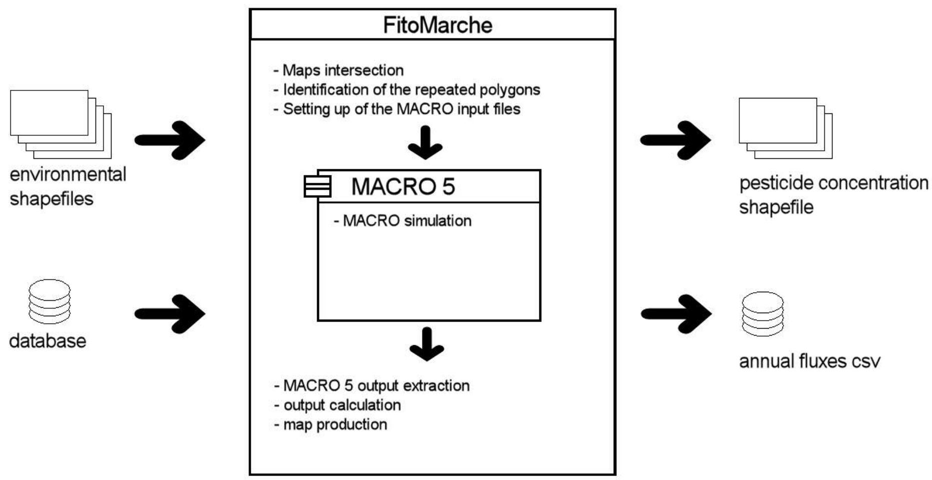
The FitoMarche software is easy to use and allows the simulation of pesticide behaviour at different scales, depending on the level of detail of input data provided as geographical layers. FitoMarche has been developed to assist regional surveys in the design of groundwater pesticide sampling strategies and in the definition of vulnerable areas at a regional scale. The need of this software was born to fulfil the request of Marche Region (Italy) to get a tool for realising their own pesticide vulnerability maps, but the use of standard file formats, yielded a product that can be used in any catchment / region.

Several tools have been already developed but no one considers crop rotations in the assessment and generally they assess pesticide behaviour by a worst case approach.

This software assesses pesticide behaviour in soil following real agronomic use and allows an analysis of variability in the use of agrochemicals, both spatially and temporally. It can be useful in defining pesticide use permissions or restrictions at a regional level or in planning monitoring programmes, optimizing the study budget by focusing sampling in the areas where higher pesticide concentrations are likely to be found.

How does the program work?

The software uses real data, scaling a 1-dimensional water and pesticide model up to the basin/regional scale in 3 dimensions.



During the development of the software, particular effort was invested in the definition of rotation. Rotation is the sequence of different crops in a field, having both a spatial (distribution of the crop in the farm fields) and a temporal (the rotation of crops in the same field) dimension. Space is modelled by GIS using data from land use repositories (i.e. Corine Land Cover project) and from a rotation map. Time is modelled on the basis of the crop sequence defined using the crop properties described in the internal database. The software can model both annual and perennial crops.

The input data has been organised using the internal database and using geographical layers (shapefiles) including active ingredients, crops, soil types, land use, rotation and climate characteristics. Once all the input data have been identified, the software intersects the shapefiles and creates a set of polygons that represent different environmental conditions. To save computational time, simulations will be performed only for polygons which differ in the value of at least one property. For these polygons, FitoMarche:

creates of the set of variables required by MACRO (stored in the memory in the first instance),

writes the input file for MACRO, using values originating from the shapefiles and the database,

copies the created file, along with the other files (such as time series) to a temporary file where the model file is stored,

starts the MACRO model using the file “management.exe”,

extracts the variables required for the creation of the FitoMarche output from the MACRO output file,

deletes files no longer required from the temporary file of the simulation.

calculates the quantity of water and pesticide flowing at 1 m depth during the year or, if the soil profile is less than 1 m deep, at the bottom of the simulated profile.

Because of MACRO considers macropores and microporse, two MACRO variables are summed calculating the water flow (WOUT, mm h^{-1} and WFLOWOUT, mm h^{-1}) and two variables are summed calculating the pesticide flow (SFLOW, g m^{-2} h^{-1} and SFLOWOUT, g m^{-2} h^{-1}) and the mean annual concentration (μg L^{-1}) is calculated dividing the cumulated annual pesticide flow per the cumulated annual water flow.

The number of MACRO simulations to be performed to create the FitoMarche output depends on the scale of simulation, on the detail of the data used, on the number of years simulated, and on the number of crop on which the agrochemical is used. In some case a single run can requires few weeks of simulation. The final result of the simulation process is a shapefile contains the 80th percentile mean annual leaching concentration and the leaching depth and a comma separated value file containing annual water and solute leaching series.

How does the program operate from the perspective of the user?

Few specific skills are required to run the software for a spatial simulation and in particular few expertises on GIS and on MACRO model are necessary. It was designed bearing in mind that the end user will be a non technical administrator and, accordingly, the software uses data that are immediately available or easy to obtain. In FitoMarche, a simulation comprises a set of input and output data related to a specific territorial context.

The use of real data leads to a shift away from the concepts of “realistic” or “worst case”, representing actual worst case risk assessments, towards the concept of “ordinary”. This concept is derived from the science of estimation that attributes a monetary value to goods. During a risk assessment or estimation procedure all of the facts, objects, circumstances, conditions, people and hypothesis involved in the assessment must be considered “ordinary”, and the circumstances or the conditions must be considered endless. Each element of the assessment must be thought of as having a “normal” and constant function, and aspects considered extraordinary or outside the concept of “ordinary” have to be excluded temporarily from the estimation (Michieli, 1993). The term “ordinary” therefore refers to events that happen with the maximum frequency and extraordinary events can only be added or removed in a second step. For this reason, GIS assessment is used only to model ordinary events, whilst specific simulations can be used to analyse extraordinary aspects.

The main application form and the five panels into which it is divided (Shapes, Rotations, Irrigations, Meteorology, Simulation) are presented in Figure 2.

The user must first select the active ingredient to be considered in the simulation, and then the shapefiles that describe the main environmental variables linked to the territory:

the domain considered (usually the border of the study region, but the user can focus on a smaller area);

the land use map, according to the Corine Land Cover 2000 legend;

the soil map, linked to the specification of the horizons within the database;

the rotations map that divides the territories into areas, each associated with a prevailing rotation;

the meteorological areal map, through which the territory considered can be divided,

Finally a further shapefile, "interdiction areas map", can be loaded. This contains descriptions of the zones or territory buffers where the public authority prohibits the use of agrochemicals.

Once the shapefile relating to the rotations has been read, the software activates either the Rotations panel or the Irrigations panel. The former associates the rotation codes, found in the shapefile, with the corresponding physical rotation found in the database. The Irrigations panel shows the irrigations associated with the crops in the selected rotations, stored in the FitoMarche database. The values initially present in this form are the default values as they exist in the database. The user can, however, modify the values of water volume [100 L ha^{-1}] and pesticide rates [g ha^{-1}].

The user can associate an irrigation event with the application of a particular active ingredient only if the active ingredient is registered for the crop under consideration.

The fourth panel, "Meteorology", is activated by the software when the shapefile of the climatic polygon areas is loaded. The software takes the number of weather stations and the data that define them. Using this form, the user must associate each meteorological station with corresponding files containing rainfall and evapotranspiration data.

Once the simulation has been fully set up, as described in the previous section, it is started by selecting the “Simulation” panel of the interface. In this panel, two visual controls are used to set the start date and end date of the simulation period. The valid range of the start and end dates is set during climate file association: FitoMarche reads the date ranges from each file and uses the minimum range as the valid time period. The user may shorten the simulation period in this panel in order to reduce simulation time but, at the same time, limiting the accuracy of the result.

Once the time period has been set, the simulation can be started by clicking “Start” on the Simulation panel

The user can visualize, modify or remove different database entities by the administration tool. The tool facilitates actions relating to crops, divided into annuals and perennials, active ingredients, crops and irrigations associated with every rotation and soil profiles. The “Rotations” window deserves particular attention, since each rotation includes irrigation and treatment information. It is possible to associate one or more irrigations to each crop (therefore to each year of the rotation) and to associate the application of agrochemicals to the crop during the simulation phase. The form “Profiles” allows the user to add, remove or modify the soil profiles in the database and the horizons associated with them.