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Sabine-Karen Lammoglia, David Makowski, Julien Moeys, Eric Justes, Enrique Barriuso, et al.. Sensitivity analysis of the STICS-MACRO model to identify cropping practices reducing pesticides losses. *Science of the Total Environment*, 2017, 580, pp.117-129. 10.1016/j.scitotenv.2016.10.010 . hal-04809766

**HAL Id: hal-04809766**

**<https://hal.inrae.fr/hal-04809766v1>**

Submitted on 28 Nov 2024

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# Sensitivity analysis of the STICS-MACRO model to identify cropping practices reducing pesticides losses

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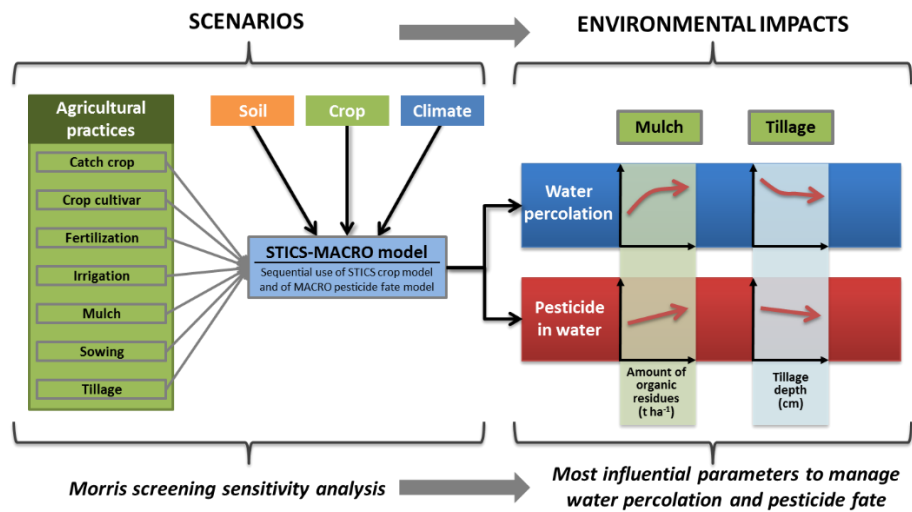
**Lammoglia SK, Makowski D, Moeys J, Justes E, Barriuso E, Mamy L, 2017.** Sensitivity analysis of the STICS-MACRO model to identify cropping practices reducing pesticides losses. **Science of the Total Environment, 580: 117-129.**

<https://doi.org/10.1016/j.scitotenv.2016.10.010>

## HIGHLIGHTS

- STICS-MACRO simulates the effects of cropping practices on water and pesticide losses
- A sensitivity analysis was performed on STICS-MACRO to identify influential cropping practices
- Mulch could increase pesticide leaching in relation to its effect on soil moisture
- A decrease in pesticides concentrations in water was simulated under soil tillage
- Effects of cropping practices on pesticide losses could be more important than those of soil, crop or climate conditions in some situations

## GRAPHICAL ABSTRACT



## ABSTRACT

STICS-MACRO is a process-based model simulating the fate of pesticides in the soil-plant system as a function of agricultural practices and pedoclimatic conditions. The objective of this work was to evaluate the influence of crop management practices on water and pesticide flows in contrasted environmental conditions. We used the Morris screening sensitivity analysis method to identify the most influential cropping practices. Crop residues management and tillage practices were shown to have strong effects on water percolation and pesticide leaching. In particular, the amount of organic residues added to soil was found to be the most influential input. The presence of a mulch could increase soil water content so water percolation and pesticide leaching. Conventional tillage was also found to decrease pesticide leaching, compared to no-till, which is consistent with many field observations. The effects of the soil, crop and climate conditions tested in this work were less important than those of cropping practices. STICS-MACRO allows an *ex ante* evaluation of cropping systems and agricultural practices and of the related pesticides environmental impacts.

*Keywords:* STICS-MACRO model, Morris sensitivity analysis, conservation agriculture, sustainable cropping practices, water percolation, pesticide leaching

## 1. Introduction

One of the current challenges of sustainable agriculture is to reduce the environmental impacts due to pesticides and to protect the environmental resources such as soil and water. A way to achieve these objectives is to introduce new cropping systems relying on integrated pest management or low input systems (Hossard et al., 2016; Mortensen et al., 2000). However, because of the wide diversity of possible combinations of crops, agricultural practices (tillage, organic matter management, mulch...), soils, and climates, it is difficult and costly to carry out comprehensive *in situ* experiments to study the sustainability of each potential new system. An alternative is to develop and use *ex ante* simulation tools to assess numerous options and to identify the best systems.

There are few modelling tools able to quantify the environmental impacts of pesticides (i.e. concentrations in soil and water) taking into account the effects of pedoclimatic conditions, agricultural practices and cropping systems: examples are STICS-MACRO (Lammoglia et al., 2016), RZWQM (Malone et al., 2004) and STICS-Pest (Queyrel et al., 2016). The performance of RZWQM to simulate pesticide fate and transport in cropping systems was shown to be good but calibration is often necessary (Malone et al., 2004). STICS-Pest was found to be efficient to predict pesticides leaching in some contexts however it has a simplified formalism for water transfer, and the non-linear sorption is not considered despite it can be decisive to simulate the fate of pesticides in the environment, and in particular in groundwater (Beltman et al., 2008; Queyrel et al., 2016). The STICS-MACRO model combines the performances of a crop model (STICS) and of a pesticide fate model (MACRO). STICS-MACRO is thus able to simulate crop growth and development, and water and pesticides leaching, and the predictions are satisfactory despite they vary with the pedoclimatic context (Lammoglia et al., 2016).

This study aims at identifying the most influential agricultural practices to reduce pesticides losses by leaching based on a sensitivity analysis of the STICS-MACRO model. Sensitivity analysis investigates the relationship between model input and output and helps to identify the parameters which require the greatest accuracy in their determination and which require the most (or least) attention when parameterizing models (Dubus et al., 2003; Saltelli et al., 2008). In this context, this analysis will help to identify the most influential STICS-MACRO management practices related inputs on pesticides losses. Among the different existing methods of sensitivity analysis, the Morris screening method proposed by Morris (1991), and then improved by Campolongo et al. (2007), can be applied to complex models in order to rank a large number of inputs with a relatively small number of simulations (Saltelli et al., 2008).

No sensitivity analysis was previously performed to STICS-MACRO but several sensitivity analyses were conducted to MACRO and STICS separately. Those conducted on the MACRO model showed that the most

important parameter affecting the predictions of percolated water volumes was the water content defining the boundary between micropores and macropores (Dubus et al., 2003). These studies also revealed that pesticide losses were influenced by pesticides properties (sorption and degradation) and by the hydrological properties of the soil (Dubus et al., 2003; Larsbo et al., 2005; Lindahl et al., 2005). On the contrary, few global sensitivity analyses had previously been conducted on the STICS model. Ruget et al. (2002) showed that the sensitivity of STICS to the various input parameters depends on the different conditions of climate, crops and soils, and that no parameter was systematically influential. However, the crop development module of STICS was most sensitive to juvenile stage duration and filling stage duration, while the leaf area index module of STICS was most sensitive to crop density.

The effect of crop management on pesticide losses in the environment has never been studied. Therefore, in this study, we explored the effects of changes in model inputs related to crop management on the water percolation and pesticide leaching values simulated by STICS-MACRO for different soil-crop-climate conditions. Results were used to identify the most relevant cropping practices allowing reduction in pesticides losses in the environment.

## **2. Materials and methods**

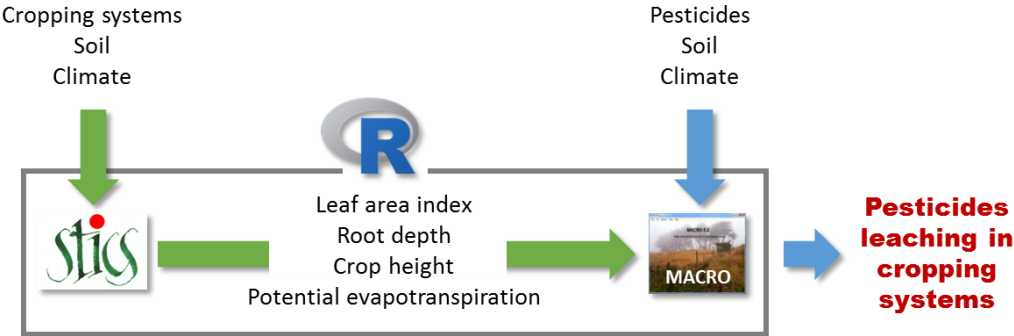
### *2.1. STICS-MACRO*

STICS (Simulateur multi disciplinaire pour les Cultures Standards, Brisson et al., 1998) is a dynamic crop model designed for site-scale operational applications, which describes in detail the soil and crop processes associated with numerous crop varieties and management practices. STICS predicts more than 200 variables, on a daily basis, related to the crop production (LAI, quantity and quality of yield), to the environment (water, carbon, and nitrogen fluxes), and to the evolution of soil water and nitrate contents. STICS has been widely tested and its performance was shown to be good to simulate many outputs such as soil water content or crop development, under various agricultural practices (Brisson et al., 2003; Coucheney et al., 2015).

MACRO (Larsbo et al., 2005) is a one-dimensional dual-permeability model of water flow and solute transport in macroporous soil. The water and solute are partitioned into two domains: micropores, where equilibrium flow and transport occur, represented by the Richards and the convection-dispersion equations, and macropores, where non-equilibrium gravity-driven flow occurs. Pesticide sorption is described using the Freundlich isotherm, while degradation is described using first-order kinetics and depends on soil temperature and moisture content. The representation of crop development is simply based on crops' emergence and harvest dates,

maximum LAI, maximum root depth and maximum crop height. No agricultural practices such as mulching or tillage can be considered. The performance of MACRO is known to be good to predict the fate of pesticides under conventional crop management (e.g. Marín-Benito et al., 2014).

STICS-MACRO results in the combined use of STICS and MACRO in order to simulate crop growth and pesticide fate in complex cropping systems (Fig. 1) (Lammoglia et al., 2016). Dedicated R packages (R Development Core Team, 2016) were developed to automate the forcing of MACRO inputs with some STICS output variables. The packages allow to sequentially (1) import predefined STICS and MACRO parameterization sets (one for each model), (2) simulate the crop rotation, crop development, water, and nitrogen requirements under agricultural practices such as fertilization or crop residues management with STICS model, (3) extract from STICS output files the estimated potential evapotranspiration, as well as the estimated green and total leaf area index, the crop height and the maximum root depth (for each time step), (4) convert these to MACRO input file format and adapt MACRO parameterization, (5) re-estimate the fraction of the sprayed pesticide intercepted by the crop based on STICS total LAI when the pesticide is sprayed, (6) run the MACRO model with crop shape variables and potential evapotranspiration coming from STICS, and finally (7) import MACRO simulation results, i.e. water balance and pesticides concentrations in soils and water as a function of time. The results can either be analyzed and visualized in R or exported. Internally, the tools use existing command line modes of STICS and MACRO, but do not use the graphical user interfaces of the two models. As indicated above, the performance of STICS-MACRO to simulate the fate of pesticides under different cropping systems was shown to be good despite they vary with the pedoclimatic context (Lammoglia et al., 2016).



**Fig. 1.** Combined use of STICS crop model and of MACRO pesticide fate model to simulate pesticides leaching in cropping systems (From Lammoglia et al., 2016).

## 2.2. STICS-MACRO crop management inputs

The sensitivity analysis aims at ranking all STICS-MACRO inputs related to crop management practices (Table 1). These inputs describe N fertilization (nitrogen stress index - *ratioLN*, fraction of ammonium in the N fertilizer - *engamm*, amount of N immobilized - *Norgeng*, maximal fraction of the mineral fertilizer that can be denitrified - *deneng*, maximum fraction of mineral fertilizer that can be volatilized - *voleng*), water supply (water stress index - *ratioI*), tillage practices and crop residues management (tillage date - *jultrav*, amount of organic residues - *qres*, water content of organic residues - *eaures*, minimal value of the depth where organic residues are incorporated - *profres*, maximum value of the depth where organic residues are incorporated - *proftrav*, C/N ratio of organic residues - *CsurNres*, proportion of N mineral content of organic residues - *Nminres*, date of addition of organic residues to soil - *julres*), and sowing operations (date of sowing - *iplt0*, plant sowing density - *densite*, depth of sowing - *profsem*). The initial water and nitrate contents of the different soil horizons (water content in each horizon - *Hinit1-5*, and nitrate content in each horizon - *Ninit1-5*) were considered in the sensitivity analysis because they are influenced by the presence or absence of a catch crop before the main crop (Table 1).

Several inputs describing cultivar characteristics were also taken into account: maximum grain weight (*pgrainmaxi*), cumulative thermal time between the end of the juvenile phase and the end of leaf growth (*stamflax*), cumulative thermal time between the starting date of filling of harvested organs and the physiological maturity (*stdrpmat*), cumulative thermal time between the maximum LAI and the leaf senescence (*stlaxsen*), cumulative thermal time between the emergence and the end of juvenile phase (*stlevamf*), and cumulative thermal time between the leaf senescence and LAI zero (*stsenlan*).

Therefore, a total of 33 inputs were considered. Their ranges of variation were based on measurement, literature review or experts' recommendations (Table 1).

**Table 1.** STICS inputs (Ripoche-Wachter and Cufi, 2013) used in the sensitivity analysis and their ranges of variation

Symbol	Description	Parameter	Unit	Maize		Winter wheat	
				Min	Max	Min	Max
CsurNres <sup>b,d</sup>	C/N ratio of organic residues		(-)	10	125	10	125
deneng <sup>a</sup>	Maximal fraction of the mineral fertilizer that can be denitrified		(-)	0.05	0.2	0.05	0.2
densite <sup>a</sup>	Plant sowing density		plants/m <sup>2</sup>	5	20	200	400
eaures <sup>a,d</sup>	Water content of organic residues		% fresh weight	0	100	0	100
engamm <sup>a</sup>	Fraction of ammonium in the N fertilizer		(-)	0.5	1	0.5	1
Hinit1 <sup>a</sup>	Initial water content of the first soil horizon		%	0	30	0	30
Hinit2 <sup>a</sup>	Initial water content of the second soil horizon		%	0	30	0	30
Hinit3 <sup>a</sup>	Initial water content of the third soil horizon		%	0	30	0	30
Hinit4 <sup>a</sup>	Initial water content of the fourth soil horizon		%	0	30	0	30
Hinit5 <sup>a</sup>	Initial water content of the fifth soil horizon		%	0	30	0	30
iplt0 <sup>a</sup>	Date of sowing		Julian day	90 (Early)	129 (Late)	275 (Early)	323 (Late)
julres <sup>a</sup>	Date of organic residues addition to soil		Julian day	iplt0 - 14	iplt0 - 2	iplt0 - 14	iplt0 - 2
jultrav <sup>a</sup>	Date of soil tillage		Julian day	iplt0 - 14	iplt0 - 2	iplt0 - 14	iplt0 - 2
Ninit1 <sup>a</sup>	Initial NO <sub>3</sub> content in the first soil horizon		kgN ha <sup>-1</sup>	0	30	0	30
Ninit2 <sup>a</sup>	Initial NO <sub>3</sub> content in the second soil horizon		kgN ha <sup>-1</sup>	0	30	0	30
Ninit3 <sup>a</sup>	Initial NO <sub>3</sub> content in the third soil horizon		kgN ha <sup>-1</sup>	0	30	0	30
Ninit4 <sup>a</sup>	Initial NO <sub>3</sub> content in the fourth soil horizon		kgN ha <sup>-1</sup>	0	30	0	30
Ninit5 <sup>a</sup>	Initial NO <sub>3</sub> content in the fifth soil horizon		kgN ha <sup>-1</sup>	0	30	0	30
Nminres <sup>a,d</sup>	Proportion of N mineral content of organic residues		% fresh weight	0	10	0	10
Norgeng <sup>a</sup>	Amount of N immobilized		kgN ha <sup>-1</sup>	0.2	42	0.2	42
pgrainmaxi <sup>a</sup>	Maximum grain weight		g	0.24	0.36	0.24	0.36
profres <sup>c,d</sup>	Minimal value of the depth where organic residues are incorporated		cm	0	30	0	30
profsem <sup>b,d</sup>	Depth of sowing		cm	1	10	1	10
proftrav <sup>b,d</sup>	Maximum value of the depth where organic residues are incorporated		cm	0	30	0	30
qres <sup>b,d</sup>	Amount of organic residues added to soil		t ha <sup>-1</sup>	0	30	0	30
ratioI <sup>a</sup>	Water stress index below which irrigation is started in automatic mode		(-)	0.2	1	0.2	1
ratioIN <sup>a</sup>	Nitrogen stress index below which fertilization is started in automatic mode		(-)	0.2	1	0.2	1
stamflax <sup>a</sup>	Cumulative thermal time between the AMF <sup>e</sup> and LAX <sup>e</sup> stages		Degree.day	390	600	390	600
stdrpmat <sup>a</sup>	Cumulative thermal time between the DRP <sup>e</sup> and MAT <sup>e</sup> stages		Degree.day	570	780	570	780
stlaxsen <sup>a</sup>	Cumulated thermal time between the LAX <sup>e</sup> and SEN <sup>e</sup> stages		Degree.day	680	800	680	800
stlevamf <sup>a</sup>	Cumulated thermal time between the LEV <sup>e</sup> and AMF <sup>e</sup> stages		Degree.day	190	310	190	310
stsenlan <sup>a</sup>	Cumulated thermal time between the SEN <sup>e</sup> and LAN <sup>e</sup> stages		Degree.day	180	300	180	300
voleng <sup>a</sup>	Maximum fraction of mineral fertilizer that can be volatilized		(-)	0	0.35	0	0.35

<sup>a</sup> From expert judgement; <sup>b</sup> From Ruget et al. (2002); <sup>c</sup> Limits imposed by STICS; <sup>d</sup> The same values will be used for the two crops; <sup>e</sup> AMF: Maximum acceleration of leaf growth, end of juvenile phase; LAX: Maximum leaf area index, end of leaf growth; DRP: Starting date of filling of harvested organs; MAT: Physiological maturity; SEN: Beginning of leaf senescence; LEV: Emergence; LAN: Leaf index zero



### *2.3. Definition of the scenarios*

The combination of two soils, two crops, and two climates resulted in eight scenarios.

#### *2.3.1. Soils*

Two soils were selected differing in depth, physical and hydraulic characteristics (Table 2). The Dijon soil is a clayey calcic Cambisol (FAO, 2014), and the Lamothe soil is a stagnic Luvisol (FAO, 2014) with an illuvial clay horizon between 35 and 60 cm. The soil hydraulic parameters, such as the soil water contents at wilting point and at field capacity, the saturated water content, the residual water content, the van Genuchten's soil-water retention parameters, the saturated hydraulic conductivity, the boundary (i.e. between macropores and micropores) soil water tension, the boundary hydraulic conductivity and the boundary water content were estimated using RETC (RETention Curve) (Van Genuchten et al., 1991) (Table 2).

#### *2.3.2. Crops*

Two crops have been considered for each soil: one winter crop (winter wheat) and one spring crop (maize). They were selected for the following reasons: (i) they cover different pesticide application periods (in November for winter wheat and in May for maize); (ii) they have contrasted growing season lengths and water requirements; (iii) wheat and maize are the most cultivated crop in France with a sowing area about 5 million ha and 1.85 million ha, respectively (Agreste, 2015).

#### *2.3.3. Climates*

The daily values of rainfall, air temperature, global solar radiation, relative humidity and wind speed were obtained from the Dijon meteorological station of INRA (Climatik, 2016). From 1996 to 2015, the mean annual rainfall is 744 mm, and the mean annual temperature is 11.3 °C. Among these 20 years, two climatic years were selected to test the impact of different precipitation regimes on the results: one dry year, corresponding to 2003, with a low annual rainfall of 623 mm and a mean temperature of 12.1 °C; and one wet year corresponding to 2013, with an annual rainfall of 940.5 mm and a mean temperature of 10.7 °C.

**Table 2.** Dijon and Lamothe soils physicochemical and hydraulic characteristics

	Dijon			Lamothe				
	0-21	21-44	44-100	0-10	10-30	30-60	60-100	100-200
Depth (cm)	0-21	21-44	44-100	0-10	10-30	30-60	60-100	100-200
Clay (%) <sup>a</sup>	39.1	44.4	49.4	32.2	34.6	35.5	43.8	33.9
Silt (%) <sup>a</sup>	55.1	50.7	44.1	45.2	42.8	44.0	39.4	22.1
Sand (%) <sup>a</sup>	5.8	4.9	6.5	22.6	22.6	20.5	16.8	44
Organic carbon (%) <sup>a</sup>	1.86	1.14	0.63	1.38	1.07	0.95	0.71	0.24
pH (water) <sup>a</sup>	7.01	7.26	7.93	6.68	6.40	7.13	7.76	7.87
Bulk density (g cm <sup>-3</sup> ) <sup>a</sup>	1.44	1.44	1.48	1.50	1.50	1.56	1.63	1.63
Soil water content at wilting point (m <sup>3</sup> m <sup>-3</sup> ) <sup>a</sup>	0.134	0.148	0.158	0.114	0.12	0.122	0.146	0.142
Soil water content at field capacity (m <sup>3</sup> m <sup>-3</sup> ) <sup>b</sup>	0.298	0.306	0.308	0.27	0.273	0.27	0.28	0.26
Saturated water content (m <sup>3</sup> m <sup>-3</sup> ) <sup>b</sup>	0.46	0.505	0.456	0.414	0.419	0.406	0.399	0.381
Boundary water content (m <sup>3</sup> m <sup>-3</sup> ) <sup>b</sup>	0.405	0.390	0.424	0.411	0.415	0.402	0.394	0.373
Residual water content (m <sup>3</sup> m <sup>-3</sup> ) <sup>b</sup>	0.092	0.102	0.095	0.08	0.083	0.081	0.084	0.071
Alpha van Genuchten parameter (cm <sup>-1</sup> ) <sup>b</sup>	0.01	0.0125	0.013	0.010	0.011	0.011	0.014	0.020
n van Genuchten parameter (-) <sup>b</sup>	1.439	1.390	1.335	1.464	1.434	1.409	1.307	1.258
saturated hydraulic conductivity (m d <sup>-1</sup> ) <sup>b</sup>	0.064	0.139	0.050	0.528	1.560	0.24	0.024	0.024
boundary hydraulic conductivity (m d <sup>-1</sup> ) <sup>b</sup>	0.001	0.004	0.017	0.014	0.024	0.034	0.007	0.026
boundary soil water tension (cm) <sup>c</sup>	40	40	50	10	10	10	10	10
effective diffusion pathlength (mm) <sup>d</sup>	5	5	5	6	6	30	30	20
ZN tortuosity/pore size distribution factor (-) <sup>c</sup>	2	2	2	3	3	2	2	2

<sup>a</sup> Parameters that were directly measured in laboratory; <sup>b</sup> Estimated with RETC (RETention Curve) (Van Genuchten et al., 1991); <sup>c</sup> Estimated from Beulke et al. (2002); <sup>d</sup> Estimated using MACRO 5.0/5.1 pedotransfer function

### 2.3.4. Pesticide

The selected pesticide was the Dummy B substance of FOCUS (2000). This pesticide has a low persistence (DT50 = 20 days), but a high mobility ( $K_{oc} = 17 \text{ L kg}^{-1}$ ) (Table 3), and can lead to significant leaching of the compound at 1 m depth which is the endpoint considered at the European regulatory level (FOCUS, 2000; Regulation EC No 1107/2009, 2009). The fraction of sorption sites attributed to the macropore (FRACMAC), as needed in MACRO, was set to 0.02 (Dubus et al., 2003). For all scenarios, the pesticide was applied at a rate of  $1 \text{ kg ha}^{-1}$ . For the winter wheat, it was sprayed the 1 November (Julian day 305); for the spring crop, maize, it was sprayed the 5 May (Julian day 125). Pesticide fate and transport were simulated with constant soil hydraulic properties.

**Table 3.** Soil adsorption coefficients ( $K_{oc}$ ) and half-lives (DT50) of the Dummy B substance (FOCUS, 2000) in Dijon and Lamothe soils profiles

Dijon			Lamothe		
Depth (cm)	$K_{oc}$	DT50 (days)	Depth (cm)	$K_{oc}$	DT50 (days)
0-21 <sup>a</sup>	17	20	0-10 <sup>a</sup>	17	20
21-30 <sup>b</sup>	10.42	20	10-30 <sup>b</sup>	13.18	20
30-44 <sup>b</sup>	10.42	40	30-60 <sup>b</sup>	11.7	40
44-60 <sup>b</sup>	5.76	40	60-100 <sup>b</sup>	8.75	67
60-100 <sup>b</sup>	5.76	67	100-200 <sup>b</sup>	2.96	No degradation

<sup>a</sup> From FOCUS (2000); <sup>b</sup> Variation of DT50 with depth was determined according to FOCUS (2000), and that of  $K_{oc}$  was determined according to soil organic carbon content (Table 2)

### 2.3.5. Outputs

For each combination of soil-crop-climate, the model sensitivity was analyzed for three outputs of STICS-MACRO: (i) one year cumulative amount of water at 1 m depth starting at the pesticide application date; (ii) total amount of pesticide at 1 m depth during one year after the pesticide application date; (iii) daily maximum concentration of pesticide at 1 m depth.

## 2.4. Sensitivity analysis

The sensitivity analysis was based on the method of Morris (Campolongo et al., 2007; Morris, 1991). Like all screening methods, the Morris method provides qualitative information on the sensitivity of the outputs to the set of inputs, since it only discriminates inputs based on their importance, but does not provide information on the relative difference of importance (Cariboni et al., 2007). It allows inputs to be ranked and classified as (i) negligible, (ii) linear and additive, or (iii) non-linear or non-additive due to interactions with other inputs

(Campolongo et al., 2007; Saltelli et al., 2008). Its advantage is that it requires relatively few model evaluations and does not assume or require any particular model structure (e.g. linearity).

The Morris experimental design is based on individually randomized one-at-a-time experiments (Campolongo et al., 2007) in which two successive evaluations of the model differ by only one input. The values of each quantitative input  $x_i$  ( $i = 1$  to  $k$  where  $k = 33$ ) are standardized with their minimal and maximal values to vary in  $\{0, 1\}$  intervals. These  $\{0, 1\}$  intervals are then divided into  $p$  equispaced values or levels. A sampling procedure is used to generate trajectories in the input space (Campolongo et al., 2007). The  $r$  trajectories define the intensity with which the parameter space is explored. From each repetition  $j$  ( $j = 1$  to  $r$ ), the Morris method computes an elementary effect ( $EE_i^{(j)}$ ) at the  $j^{\text{th}}$  repetition, resulting for a change of size  $\Delta$  of the  $i^{\text{th}}$  input on the output, as follows:

$$EE_i^{(j)} = \frac{f(x_1, \dots, x_{i-1}, x_i + \Delta, x_{i+1}, \dots, x_k) - f(x)}{\Delta} \quad (1)$$

where  $k = 33$  is the number of input parameters;  $x_1, \dots, x_i, x_i + \Delta, x_k$  take values in the set  $\{1 / (p - 1), 2 / (p - 1), \dots, 1 - 1 / (p - 1)\}$ ; and  $p$  is the number of levels (see below). A value of  $EE_i$  is calculated for each input in turn. Each trajectory is thus defined by the values of  $EE_i$  calculated for the  $k = 33$  inputs.

Two sensitivity indices are computed from the values of the elementary effects (Morris, 1991),  $\mu_i$  and  $\sigma_i$ , which evaluate the overall effect of each input  $x_i$  on the model output, and the parameters' higher order effects caused by non-linear input effect and by interactions between inputs, respectively (Campolongo et al., 2007). For each input  $x_i$ , the  $\mu_i$  and  $\sigma_i$  indices are the mean and the standard deviation of the  $r$  elementary effects (see equations 2 to 4). A potential drawback of using  $\mu_i$  to gauge parameter importance is that in some cases, negative and positive values of  $EE_i$  can essentially cancel each other out when calculating the mean, and the resulting diminished  $\mu_i$  value could lead to an undervaluation of the parameter's significance. Therefore, Campolongo et al. (2007) improved the estimation of  $\mu_i$  by  $\mu_i^*$  with the absolute value  $EE_i$ :

$$\mu_i = \frac{1}{r} \sum_{j=1}^r EE_i^{(j)} \quad (2)$$

$$\mu_i^* = \frac{1}{r} \sum_{j=1}^r |EE_i^{(j)}| \quad (3)$$

$$\sigma_i = \sqrt{\frac{1}{r-1} \sum_{j=1}^r [EE_i^{(j)} - \mu_i]^2} \quad (4)$$

A large  $\mu_i^*$  value indicates that  $x_i$  is influential to the considered model output, whereas a large  $\sigma_i$  value indicates a strong non-linear or interactive relationship between  $x_i$  and the other parameters. Here, we used the Morris method as implemented in the R ‘‘Sensitivity’’ package (R Development Core Team, 2016).

Before the application of Morris screening, two parameters have to be defined: the level number  $p$  and the trajectories number  $r$ . According to Campolongo et al. (2007),  $r$  should be chosen between 10 and 50. Saltelli et al. (2008) observed that good results are often obtained with  $p = 4$  ( $\Delta = 2/3$ ) and  $r = 10$ . Vanuytrecht et al. (2014) found that the ranking achieved with 25 trajectories was similar to the ranking achieved with 400 trajectories. In this work, the number of levels  $p$  was equal to 4 and  $r$  was set equal to 50. With this setting, for each scenario, a total of 1700 inputs combinations were evaluated within the ranges shown in Table 1. Over the 8 scenarios, a total of 13600 simulations were run. The inputs were classified in three categories: “highly influential” if  $\mu^* > 0.5 \mu_{max}^*$ , “influential” if  $0.1 \mu_{max}^* < \mu^* < 0.5 \mu_{max}^*$ , parameters with  $\mu^* < 0.1 \mu_{max}^*$  having low or negligible impact.

#### 2.4. Statistical analysis

Significant differences among the rankings obtained for the eight scenarios were determined with the non-parametric test of Kruskal-Wallis. Data normality was first tested using the Shapiro-Wilk test at  $P < 0.05$  but the distribution of the data was found not to present the homogeneity of variance and the normal distribution required to do an ANOVA. The Kruskal-Wallis analyses were performed at the significance level  $P = 0.05$  with the R software (R Development Core Team, 2016).

The test of Kruskal-Wallis was also used to study the effect of different values of each influential input on the model outputs. Indeed, each input value is simulated several times thus providing a set of values for the considered output. This set of values or group is compared to the groups obtained for the other values of the same input. This comparison will allow us to determine the relative importance of each input, then to identify how each input influences the considered output.

The software package used for the statistical analysis was the Dunn-Test of R (R Development Core Team, 2016).

### 3. Results and discussion

#### 3.1. Influential crop management inputs on STICS-MACRO environmental outputs

The Morris screening method was used to qualitatively identify the parameters having the most important influence on the selected outputs of STICS-MACRO: the total amount of percolated water, the total amount of leached pesticide and the maximum concentration of pesticide.

### 3.1.1. Water percolation

For water percolation, the “highly influential” parameters ( $\mu^* > 0.5 \mu^*_{max}$ ) were mostly related to the mulch of crop residues and to the tillage practices (Fig. 2): amount of organic residues added to soil (*qres*), water content of organic residues (*eaures*), maximum value of the depth where organic residues are incorporated (*proftrav*), date of organic residues addition to soil (*julres*), and date of soil tillage (*jultrav*). It has to be noted that *qres* and *eaures* are correlated as STICS considers the dry weight of organic residues to simulate their fate (*qres* can either be set as fresh weight with a corresponding value for *eaures* or as dry weight with *eaures* set to 0). The *eaures* only plays a role in case of manure residues for the simulation of ammonia volatilization: the volatilization decreases when *eaures* increases which increases the amount of mineral nitrogen in the soil (Brisson et al., 2008). Two other “highly influential” parameters were related to sowing (depth - *profsem* and date - *iplt0*), and one to irrigation (water stress index below which irrigation is started in automatic mode - *ratioI*) (Fig. 2). These results were similar for all scenarios.

The “influential” parameters ( $0.1 \mu^*_{max} < \mu^* < 0.5 \mu^*_{max}$ ) were mainly related to the cultivar (cumulative thermal time between the end of the juvenile phase and the end of leaf growth - *stamflax*, cumulative thermal time between the starting date of filling of harvested organs and the physiological maturity - *stdrpmat*, cumulative thermal time between the emergence and the end of juvenile phase - *stlevamf*, and maximum grain weight - *pgrainmaxi* which is important for maize crop), but also to organic residues (C/N ratio of residues - *CsurNres*, proportion of N mineral content of organic residues - *Nminres*), and to sowing (plant sowing density - *densite*) (Fig. 2). The initial water contents of the five soil horizons (*Hinit1-5*) were also found influential parameters (Fig. 2).

Depending on the scenario, from 13 to 24 parameters (39 to 73% of the parameters) had low or negligible impact ( $0 < \mu^* < 0.1 \mu^*_{max}$ ) on water percolation (Fig. 2). Parameters that are common for all scenarios are related to the soil nitrate content before the sowing of the main crop and to the crop fertilization: initial nitrate contents of the five soil horizons (*Ninit1-5*), nitrogen stress index (*ratioIN*), ammonium in fertilizer (*engamm*), amount of N immobilized (*Norgeng*), proportion of denitrified fertilizer (*deneng*), and volatilized fertilizer (*voleng*) (Fig. 2).



Finally, two parameters were found to have no impact ( $\mu^* = 0$ ) whatever the environmental conditions were: cumulative thermal time between the maximum LAI and the leaf senescence (*stlaxsen*), and cumulative thermal time between the leaf senescence and LAI zero (*stsenlan*). For maize in Lamothe soil scenario, initial nitrate (*Ninit<sub>5</sub>*) and water (*Hinit<sub>5</sub>*) contents of the deepest soil horizon were not influential, and for wheat crop sowed under wet climate scenario, nitrogen stress (*ratiolN*), ammonium in fertilizer (*engamm*), amount of N immobilized (*Norgeng*), proportion of denitrified fertilizer (*deneng*), and volatilized fertilizer (*voleng*) had no impact.

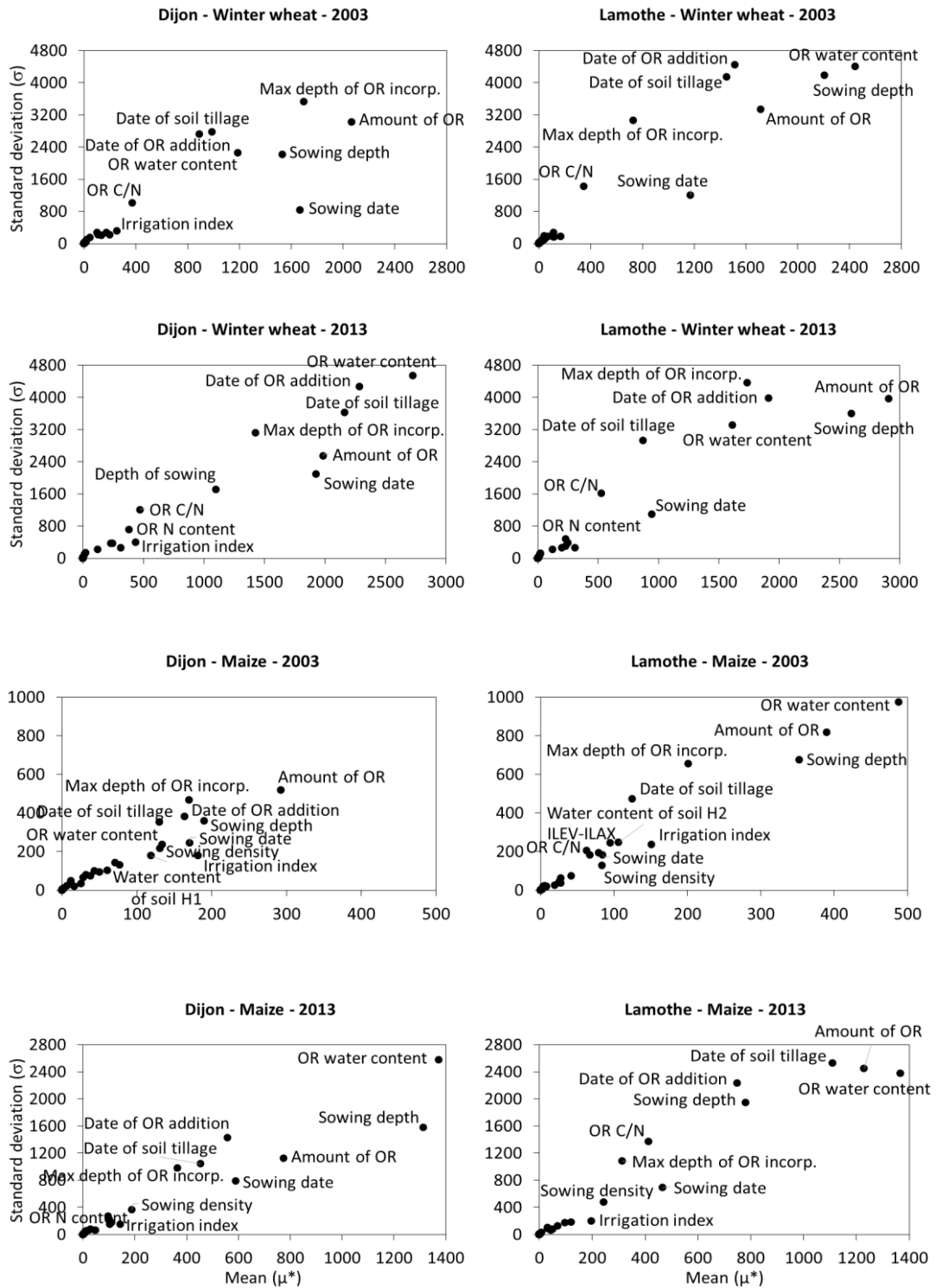
### 3.1.2. Pesticide leaching

The total amount of leached pesticide was affected by the same “highly influential” and “influential” parameters as the total amount of percolated water, but with some differences in the order of their importance (Fig. 3).

The strong correspondence between parameters affecting water percolation and pesticide leaching reflects the way STICS and MACRO are linked. Indeed, in STICS-MACRO, the LAI values are involved in the calculation of the amount of pesticide reaching the soil after interception by the crop (Lammoglia et al., 2016). The daily LAI increment is calculated as a function of heat unit sum and development phase but also of water and nitrogen limitation indices. The impact of STICS parameters on the amount of solute leached occurs through their effects on processes related to LAI.

Depending on the scenario, from 16 to 25 parameters (48 to 76% of the parameters) had low or negligible impact on pesticide leaching. As for percolated water, those parameters were mainly related to fertilization and included nitrogen stress index (*ratiolN*), ammonium in fertilizer (*engamm*), amount of N immobilized (*Norgeng*), proportion of denitrified fertilizer (*deneng*), volatilized fertilizer (*voleng*), initial nitrate contents of the soil horizons (*Ninit<sub>1-5</sub>*), proportion of N mineral content of organic residues (*Nminres*), C/N ratio of residues (*CsurNres*), but also of the minimal value of the depth where organic residues are incorporated (*profres*), plant sowing density (*densite*), water stress index below which irrigation is started in automatic mode (*ratiol*), maximum grain weight (*pgrainmaxi*), cumulative thermal time between the starting date of filling of harvested organs and the physiological maturity (*stdrpmat*), cumulative thermal time between the end of the juvenile phase and the end of leaf growth (*stamflax*), and cumulative thermal time between the emergence and the end of juvenile phase (*stlevamf*).





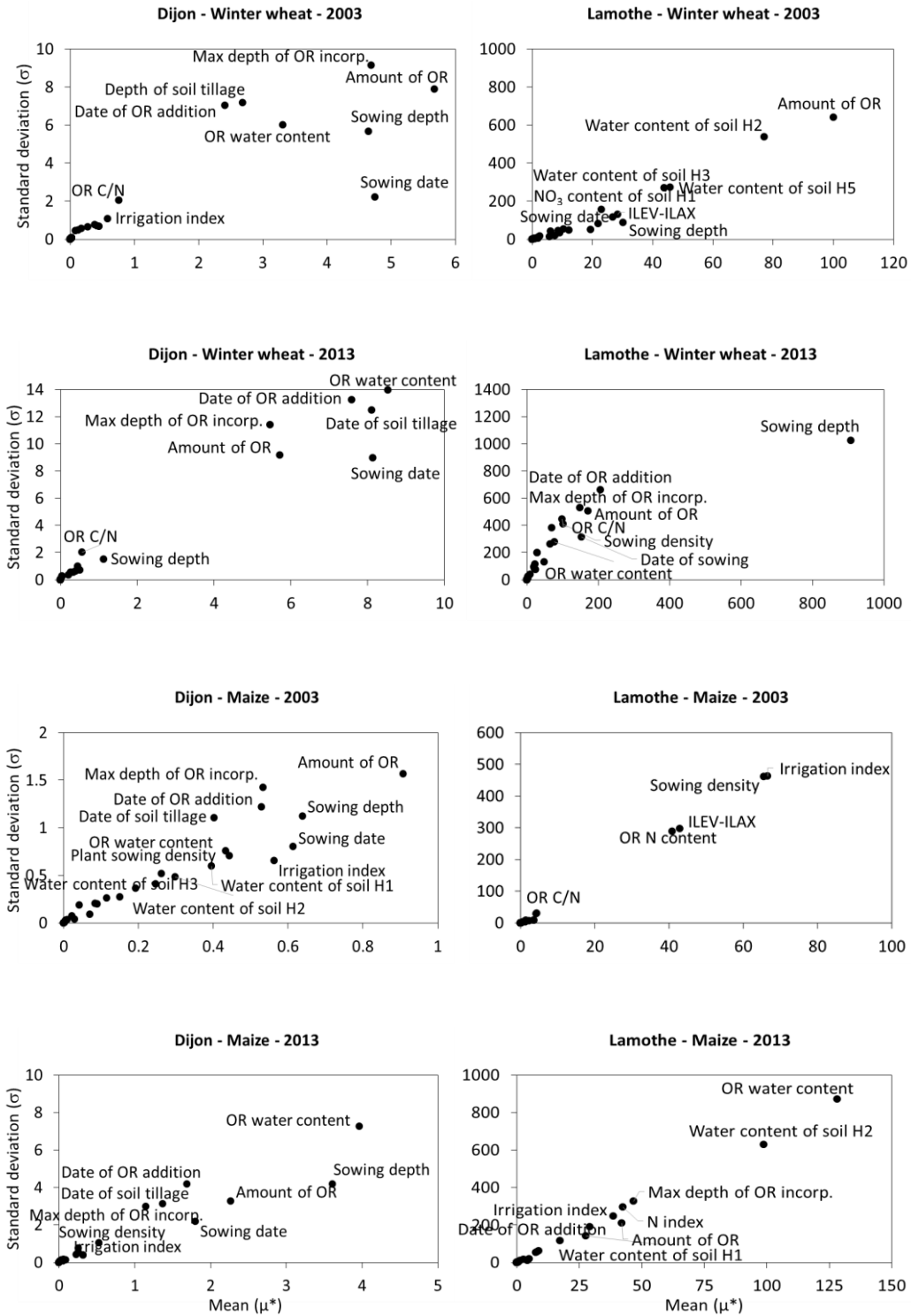
**Fig. 3.** Scatter plots of the results of the Morris sensitivity analysis. The  $\mu^*$  and  $\sigma$  are the mean and the standard deviation of the elementary effects. The graph shows the sensitivity of the model output “cumulative amount of pesticide at 1 m depth” to the following inputs:  $H_i$ , soil horizon  $i$ ; ILEV-ILAX, cumulative thermal time between the stages “emergence” and “maximum acceleration of leaf growth, end of juvenile phase”; Irrigation index, water stress index below which irrigation is started in automatic mode; OR, organic residues.

### 3.1.3. Maximum pesticide concentration

In general, the maximum pesticide concentration was influenced by the 8 “highly influential” parameters affecting the total amount of percolated water and the total amount of leached pesticide (Fig. 4). However, for Lamothe soil, the results were slightly different as “highly influential” parameters were found to be: plant sowing density (*densite*), proportion of N mineral content of organic residues (*Nminres*), initial water content of the second soil horizon (*Hinit<sub>2</sub>*), and cumulative thermal time between the emergence and the end of juvenile phase (*stlevamf*) (Fig. 4).

Eleven parameters were found “influential”: they were related to organic residues (C/N ratio of organic residues - *CsurNres*), fertilization (proportion of N mineral content of organic residues - *Nminres*, initial mineral nitrogen content in the first soil horizon - *Ninit<sub>1</sub>*, nitrogen stress index below which fertilization is started in automatic mode - *ratiolN*), sowing (plant sowing density - *densite*), and initial water content in the five soil horizons (*Hinit<sub>1-5</sub>*). Nine of these eleven parameters also influenced the total amount of percolated water and the total amount of leached pesticide (Fig. 4). The initial mineral nitrogen content in the first soil horizon (*Ninit<sub>1</sub>*) and the nitrogen stress index below which fertilization is started in automatic mode (*ratiolN*) were only “influential” in the Lamothe soil (Fig. 4).

Seventeen to twenty-nine parameters (51 to 88% of the parameters) had low or negligible impact on maximum pesticide concentration. They included all the parameters that had low or negligible impact on water percolation or pesticide leaching, and some parameters previously identified as “highly influential”: amount of organic residues (*qres*), maximum value of the depth where organic residues are incorporated (*proftrav*), date of sowing (*iplt0*), depth of sowing (*profsem*), and date of soil tillage (*jultrav*).



**Fig. 4.** Scatter plots of the results of the Morris sensitivity analysis. The  $\mu^*$  and  $\sigma$  are the mean and the standard deviation of the elementary effects. The graph shows the sensitivity of the model output “cumulative amount of percolated water at 1 m depth” to the following inputs:  $H_i$ , soil horizon  $i$ ; ILEV-ILAX, cumulative thermal time between the stages “emergence” and “maximum acceleration of leaf growth, end of juvenile phase”; Irrigation index, water stress index below which irrigation is started in automatic mode; OR, organic residues)

### 3.1.4. Overall remarks on influential crop management inputs

Whatever the considered output was, there were 8 “highly influential” input parameters which stand out from this Morris sensitivity analysis based on their  $\mu^*$ : amount of organic residues added to soil (*qres*) and the related water content of organic residues (*eaures*), maximum value of the depth where organic residues are incorporated (*proftrav*), date of organic residues addition to soil (*julres*), date of soil tillage (*jultrav*), water stress index below which irrigation is started in automatic mode (*ratiol*), sowing depth (*profsem*) and sowing date (*iplt0*).

Considering the various environmental conditions, some differences in the parameters ranking and in the magnitude of the impact of each parameter were nevertheless observed. In general, the sensitivity indices were higher for Lamothe soil than for Dijon soil, and higher values occurred with wheat crop than with maize crop (Fig. 2 to 4).

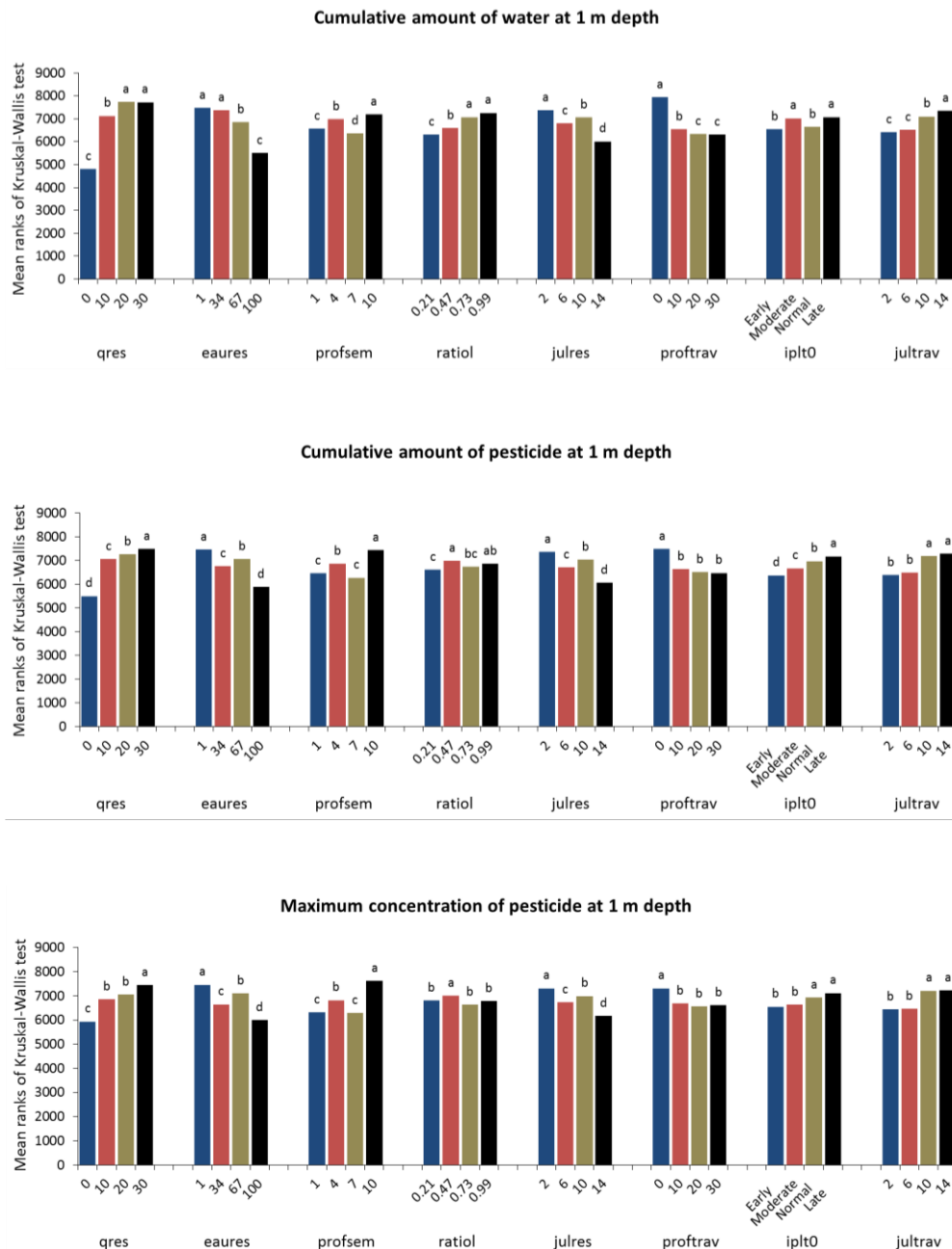
The non-linear and interactive effects between parameters reported by  $\sigma$  were also remarkable. All the subplots in Fig. 2 to 4, indicated that the 8 “highly influential” parameters with a high value of  $\mu^*$  also present a high value of the estimated standard deviation  $\sigma$ . This result means that the non-linear relationship between those inputs and model outputs was more evident than for other inputs, or that their interaction with other inputs was more noticeable. On the other hand, the input parameters with lower  $\mu^*$  also displayed lower  $\sigma$ . None of the parameters investigated showed a linear relationship, i.e. a high value of  $\mu^*$  associated with a low value of the  $\sigma$ . These results highlight that the model is strongly non-linear and non-additive.

## 3.2. Agricultural practices to manage pesticides flows in the environment

### 3.2.1. Crop residues management

The parameters controlling crop residues management practices (amount of organic residues added to soil - *qres* and the related water content of organic residues - *eaures*, and date of organic residues addition to soil - *julres*) come out consistently as the most sensitive ones controlling water percolation and pesticide leaching across the eight environmental conditions (Fig. 2 to 4).

When the amount of organic residues (*qres*) increased, a significant increase in the total amount of percolated water, total amount of pesticide, and maximum concentration of pesticide was systematically observed ( $P < 0.05$ ) (Fig. 5). A crop residue mulch of 10 t ha<sup>-1</sup> resulted in a strong increase in the water and pesticide leaching compared to the simulations with no mulch, while the effects of an additional 10 t ha<sup>-1</sup> surface residues (20 t ha<sup>-1</sup> in total) were much smaller (Fig. 5).



**Fig. 5.** Responses of cumulative amount of water at 1 m depth, cumulative amount of pesticide at 1 m depth and maximum pesticide concentration at 1 m depth to the following STICS cropping management inputs: amount of organic residues added to soil (*qres*), water content of organic residues (*eaures*), depth of sowing (*profsem*), water stress index below which irrigation is started in automatic mode (*ratiol*), date of organic residues addition to soil (*julres*), Maximal value of the depth where organic residues are incorporated (*proftrav*), date of sowing (*ipt0*), and date of soil tillage (*jultrav*). Means followed by the same letter across one parameter are not significantly different at  $P < 0.05$

The effect of *eaures* on water and pesticides flows is consistent with that of the effect of *qres*: *eaures* of 1% (dry organic residues) produced the maximum amount of percolated water and pesticide (the dry amount of organic residues is higher for *eaures* of 1% than for *eaures* of 100%) (Fig. 5). These results agree with the findings of Scopel et al. (2004) who showed, using STICS, that the presence of 6 t ha<sup>-1</sup> of surface residues more than halved soil evaporation compared to bare soil, which led to an increase in drainage. Similarly, an increase in the drainage volume of water and in pesticide concentration when surface residues were added to soil was also obtained by Shipitalo et al. (2016) who used RZWQM to simulate the fate of two herbicides in maize crop considering 0, 50 or 100% removal of maize stover.

The STICS model considers that a mulch affects soil water content through the following processes (Brisson et al., 2008): (i) the dynamic of mulch organic residues and the proportion of soil cover; (ii) the reduction in surface runoff due to the presence of obstacles on the soil surface; (iii) the rainfall interception by the mulch and its subsequent mulch direct evaporation; (iv) the radiation interception with associated reduction in soil evaporation; (v) the effects of soil evaporation and runoff on the plant's water requirements; (vi) the modifications of crop temperature linked to changes in the fluxes and albedo of the soil surface. These processes determine the evapotranspiration which is simulated by STICS considering the effect of the mulch. This evapotranspiration is then transferred to MACRO (in addition to daily crop characteristics) so that the effect of the mulch on water balance and pesticide losses can be assessed with STICS-MACRO.

The results obtained here are consistent with previous observations showing that mulch covering the soil surface directly affects soil properties such as moisture, temperature, and nutrient availability: mulch reduces soil water evaporation and runoff, it favours soil water storage and rainfall infiltration, it improves near-surface soil aggregate properties and therefore favours water percolation to deeper soil layers (Baumhardt and Jones, 2002; Blanco-Canqui and Lal, 2007; Jordán et al., 2010; Scopel et al., 2013).

According to this sensitivity analysis, no-mulch practice could induce a reduction in pesticide leaching. This suggests that, if used to control pesticide transport in the soil, mulching should not be recommended because it favours water infiltration. However, these results are in contrast with other published works demonstrating that the use of mulch is a feasible way to prevent soil and water contamination by pesticides. A mulch of crop residues may have high microbial activity, and the organic matter incorporated into the soil with the mulch can immobilize and/or enhance degradation of the pesticide and its metabolites and therefore can reduce the amount of substance that reaches the soil surface (Alletto et al., 2010). STICS-MACRO cannot simulate the change in pesticide sorption and degradation parameters due to the change in organic matter content following addition of organic residues on

the soil. However, this limit can be partially overcome by initially parameterizing STICS-MACRO with Koc and DT50 determined in organic residues amended soil. It has also to be underlined that STICS-MACRO does not consider the interception of the pesticide by the mulch that reduces the amount of substance reaching the soil (Alletto et al., 2010). But our results show that since the pesticide reaches the soil, its leaching to deeper soil layers might be enhanced because of a higher water content of soil covered by mulch. To the best of our knowledge, no experimental study has been performed to determine if the presence of a mulch could increase the leaching of pesticide already in the soil.

The effects of the mulch on water percolation and pesticide leaching also depend on the timing of the mulch addition (*julres*) (Fig. 5). When the organic residues are added 10 or 14 days before the sowing date, they induce a reduction in water percolation and in pesticide concentration. On the contrary, if the addition of organic residues is done 2 or 6 days before the sowing date, the risk of water contamination by pesticide remains high (Fig. 5). STICS simulates a significant decomposition of the mulch in the first 10 days following its addition on soil so that the remaining amount of organic residues at the sowing date is lower when applied 14 days before than 2 days before (when organic residues are added closer to the date of sowing, they are also added closer to the date of pesticide application). As indicated above, when the amount of organic residues decreases, the amounts of water and of pesticide leached at 1 m depth decrease (Fig. 5).

### 3.2.2. Tillage practices

Besides the amount and the type of residues, the results showed that the maximum value of the depth where organic residues are incorporated (*proftrav*) could greatly affect the water and pesticide flows: low depth of incorporation, so reduced-till, was found to significantly increase the water and pesticide leaching and pesticide concentration (Fig. 5). The depth of organic residues incorporation equals to 0 cm (no-till) produced the maximum pesticide concentration in the leachate (Fig. 5) independently of the environmental conditions (Supplementary data Fig. A1 to A3). Nevertheless, this effect of tillage on water and pesticide flows depends on the timing of the process through *jultrav*. When the soil tillage is done 10 or 14 days before the sowing date, it might not help to reduce pesticide concentration. On the contrary, tillage could induce a decrease in pesticide leaching when it is done 2 or 6 days before the sowing date (Fig. 5). This result remains stable among all the environmental conditions (Supplementary data Fig. A1 to A3).

The STICS model represents the effects of the soil tillage operations and of the depth of incorporation of residues in the soil through their influence on soil hydraulic conductivity and bulk density, soil temperature,

infiltration and redistribution of soil water, and available mineral nitrogen in the soil (Brisson et al., 2008). Each time the soil is tilled, STICS modelled the fragmentation of the soil due to the tillage tool, the mix of the newly added organic residues and the remix of the previous ones which are decomposing, and the modification of the environmental conditions of decomposition (temperature, soil water content, nitrogen availability). The soil fragmentation leads to a decrease in bulk density which affects soil parameters such as hydraulic conductivity, infiltrability, and water and nitrogen profiles (Brisson et al., 2008). For example, the soil tillage operations tend to increase soil evaporation by increasing its roughness. The effects of soil tillage are also taken into account through waterlogging, denitrification, nitrate leaching, root growth, and water stress.

Previous works have shown that reduced and no tillage reduce runoff and water evaporation, and enhance water infiltration and soil moisture storage (Jordán et al., 2010; Soane et al., 2012). Soil tillage affects soil structure which affects water movement via macropores. Water infiltration has been shown to occur at a faster rate under no-till than under conventional tillage because of protection by residues of the surface from raindrop impact, stability of aggregates near the surface, and continuity between the surface and sub-surface layers of vertically orientated macroporosity (Soane et al., 2012).

According to this sensitivity analysis, conventional tillage could induce a reduction in pesticide leaching. This is in agreement with the results of many authors showing that the leaching of pesticides tends to increase under no-till system (Alletto et al., 2010). STICS-MACRO simulated a greater pesticide interception by the crop (so a lower amount of pesticide reaching the soil) under conventional tillage compared with no-till practices because no-till resulted in delayed crop emergence as a result of decreased soil temperatures and increased soil water contents (Soane et al., 2012; Vetsch and Randall, 2002). Conventional tillage increased the availability of moisture for better seed germination. These results are consistent with previously published works that recorded taller plants and higher yields in conventional tillage as compared to reduced or no-till (Scopel et al., 2013; Soane et al., 2012; Vetsch and Randall, 2002).

Finally, another change related to no-till practices compared to other tillage techniques is the redistribution of organic carbon in the soil with an increase in soil surface and a gradual decrease with depth (Alletto et al., 2010; Scopel et al., 2013; Soane et al., 2012). For most pesticides, soil organic carbon content and pesticide adsorption are positively correlated. Pesticide movement can then be reduced as a consequence of a higher adsorption under conservation tillage than under conventional tillage (Alletto et al., 2010). As indicated in section 3.2.1. Crop residues management, the effect of the modification of the soil organic carbon content on pesticide adsorption following organic residues addition to soil is not considered in STICS-MACRO. However,



Steffens et al. (2015) showed that the effects of changes in soil organic carbon content of up to 3% on pesticide fate and transport as simulated by MACRO would be negligible.

### 3.2.3. Sowing practices

The results of the sensitivity analysis of STICS-MACRO also indicated that the sowing depth (*profsem*), in relation to the sowing date (*iplt0*), could affect water and pesticide flows: under crops sowed at an extreme depth of 10 cm (Arvalis, 2014), they were significantly higher than under shallow sowed crops (Fig. 5 and Supplementary data Fig. A1 to A3). Indeed, the effect of the sowing depth on water and pesticide flows occurs through the variation of the duration of crop emergence which is related to the soil temperature and moisture in the seedbed (Brisson et al., 2008). The sowing depth influences not only the duration of emergence but also the number of emerged plants. Shallow sowed seeds may germinate from a small rain while deep sowing provokes a significant delay in germination dates and seeds may die unless enough rain falls to moisten it. Germination initiates the growth of root and of shoot which may slow down with unsuitable soil moisture. If the duration between germination and emergence is too long (emergence occurs when elongation is greater than the sowing depth), there may be a reduction in plant density which can reduce the foliage production (Brisson et al., 2008). High plant density produces more foliage and quicker loss of soil moisture through transpiration leaving little water available for deep percolation. Our results seem to indicate that a sowing depth of 7 cm would help to reduce pesticide losses (Fig. 5) compared to a 4 cm depth as usually recommended (Arvalis, 2014; Arvalis, 2016). Deep sowing may also protect seeds from desiccation, rain splashing, and seed consumption by birds or rodents (Brisson et al., 1998; Pascual et al., 1999). A balance of benefits and risks would help to select the most appropriate sowing depth.

The sowing date (*iplt0*) was also shown to significantly affect water and pesticide flows (Fig. 5). The early start of the growing season generated less water and pesticide while the late start of the growing season generated higher water and pesticide. In STICS, crops development depends on the thermal index (degree.day) accumulated since the sowing date, calculated using the soil temperature at the sowing depth. Leaf area index is, up to maturity, computed as the net balance between leaf growth and senescence. Daily growth is a logistic function of development units (corresponding to the different stages) multiplied by crop efficient temperature and stress functions related to water and nitrogen limitations. Senescence occurs either when leaves reach a prescribed age or when the stress threshold related to temperature or soil water content is met (Brisson et al., 2008). Any change in LAI of the crop can affect interception of the pesticide during its application and its remobilization by rain. As early sowing dates favor crop development (e.g. Pommel et al., 2002; Spink et al., 2000), they will lead to a high

value of the LAI at the pesticide application date. From the value of the LAI, STICS-MACRO calculates the pesticide interception rate which is a key element for the assessment of pesticide concentration in water (Lammoglia et al., 2016).

#### 3.2.4. Levels of satisfaction of the crops water requirements

Irrigation is known to affect pesticide leaching (Flury, 1996). Using the automatic irrigation option, STICS calculates the water required to maintain the crops water stress index above the given threshold (*ratior*). The model then determines the irrigation schedule (the date and the amount of water applied) (Brisson et al., 2008). For a low water satisfaction level, the number of irrigations is reduced compared to a high water satisfaction level. This water satisfaction level describing irrigation calendar had a significant effect on water percolation (Fig. 5). Cropping systems which received more often irrigation water (*ratior* = 0.73 and 0.99, Fig. 5) had significantly higher water percolation ( $P < 0.05$ ) than all the other water-limited cropping systems.

When the crops water requirements are satisfied at a level of 0.21, water and pesticide leaching were found to be minimal (Fig. 5). This value corresponds to an extreme reduction in irrigation water that will induce severe crops water deficit stress. It might prevent possible pesticide losses but will greatly affect the crop yield. The percolated water increases when the satisfaction of the crops water requirements increases from 0.47 to 0.99 (Fig. 5). When *ratior* is 0.47, the amount of pesticide is maximum (Fig. 5). Although there was no significant difference between 0.73 and 0.99 levels, there was a trend toward higher water and pesticide losses from the 0.99 *ratior*. In terms of minimizing water and pesticide losses, while maintaining a good irrigation input (to get closer to the recommended ratio of 0.90), the optimum irrigation threshold would be 0.73 (Fig. 5).

## Conclusion

A Morris sensitivity analysis of the STICS-MACRO model was done to identify crop management practices that could help to decrease pesticides losses in groundwater. The results showed that water and pesticide transport could be highly affected by cropping practices, and in particular by organic residues management and by tillage. Concentrations of pesticide in leachates could decrease when there is no mulch on soil surface because the presence of mulch increases soil water content. This decrease in pesticide leaching in conventional tillage is consistent with many field observations showing that no-till favours pesticide leaching. It was also shown that the effects of cropping practices on pesticide losses could be more important than those of soil, crop or climate conditions in some situations. However, STICS-MACRO cannot simulate the changes of soil structure and of water holding

capacity of the soil following organic residues addition, and the effect of the change in soil organic carbon content on pesticide sorption and degradation. The consideration of these processes would help to improve the assessment of pesticide fate in complex cropping systems. Finally, the use of longer climatic series and of different crop rotations and soils would help to identify cropping systems allowing a decrease in the risk of pesticide leaching in various conditions.

### **Acknowledgments**

The authors are grateful to Dr. Lionel Alletto (INP-EI Purpan), Dr. Marjorie Ubertosi (AgroSup Dijon) and Dr. Nicolas Munier-Jolain (INRA) for providing soil data. This work was supported by the French Ecophyto plan, managed by the ONEMA, through two French research programs: “For the Ecophyto plan (PSPE1)” funded by the Ministry in charge of Agriculture (Perform project), and “Assessing and reducing environmental risks from plant protection products” funded by the French Ministries in charge of Ecology and Agriculture (Ecopest project). Sabine-Karen Lammoglia was supported by INRA (SMACH metaprogram) and by the Perform project.

### **Appendix A. Supplementary data**

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.scitotenv.2016.10.010>

### **References**

- Agreste, 2015. <http://agreste.agriculture.gouv.fr/IMG/pdf/memo15vegetal.pdf> (accessed 28.07.16)
- Alletto, L., Coquet, Y., Benoit, P., Heddadj, D., Barriuso, E., 2010. Tillage management effects on pesticide fate in soils. A review. *Agron. Sustain. Dev.* 30, 367-400.
- Arvalis, 2014. <http://www.arvalis-infos.fr/ma-s-semer-entre-4-et-7-cm-de-profondeur-@/view-15402-arvarticle.html> (accessed 28.07.16)
- Arvalis, 2016. Céréales et colza : Jouer la carte du progrès variétal. [http://www.arvalis-infos.fr/file/galleryelement/pj/85/8a/ca/12/atii\\_juin2016\\_16i08\\_centre1254331664067078641.pdf](http://www.arvalis-infos.fr/file/galleryelement/pj/85/8a/ca/12/atii_juin2016_16i08_centre1254331664067078641.pdf) (accessed 28.07.16)
- Baumhardt, R.L., Jones, O.R., 2002. Residue management and paratillage effects on some soil properties and rain infiltration. *Soil Till. Res.* 65, 19-27.
- Blanco-Canqui H., Lal, R., 2007. Soil structure and organic carbon relationships following 10 years of wheat straw management in no-till. *Soil Till. Res.* 95, 240-254.

- Beltman, W.H.J., Boesten, J.J.T.I., van der Zee, S.E.A.T.M., 2008. Spatial moment analysis of transport of nonlinearly adsorbing pesticides using analytical approximations. *Water Resour. Res.* 44, W05417.
- Beulke, S., Renaud, F., Brown, C., 2002. Development of guidance on parameter estimation for the preferential flow model MACRO 4.2. Final Report of the DEFRA project PL0538. Cranfield Centre for EcoChemistry, University of Cranfield, UK
- Brisson, N., Mary, B., Ripoche, D., Jeuffroy, M.H., Ruget, F., Nicoullaud, B., Gate, P., Devienne-Barret, F., Antonioletti, R., Durr, C., Richard, G., Beaudoin, N., Recous, S., Tayot, X., Plenet, D., Cellier, P., Mchet, J.M., Meynard, J.M., Delécolle, R., 1998. STICS: a generic model for the simulation of crops and their water and nitrogen balances. I. Theory and parameterization applied to wheat and corn. *Agronomie* 18, 311-346.
- Brisson, N., Gary, C., Justes, E., Roche, R., Mary, B., Ripoche, D., Zimmer, D., Sierra, J., Bertuzzi, P., Burger, P., Bussi re, F., Cabidoche, Y.M., Cellier, P., Debaeke, P., Gaudill re, J.P., H nault, C., Maraux, F., Seguin, B., Sinoquet, H., 2003. An overview of the crop model STICS. *Eur. J. Agron.* 18, 309-332.
- Brisson, N., Launay, M., Mary, B., Beaudoin, N., 2008. Conceptual Basis, Formalisations and Parameterization of the STICS Crop Model, Qu , Versailles.
- Campolongo, F., Cariboni, J., Saltelli, A., 2007. An effective screening design for sensitivity analysis of large models. *Environ. Model. Soft.* 22, 1509-1518.
- Cariboni, J., Gatelli, D., Liska, R., Saltelli, A., 2007. The role of sensitivity analysis in ecological modelling. *Ecol. Model.* 203, 167-182.
- Climatik, 2016. <https://internet.inra.fr/climatik/> (accessed 01.07.16)
- Coucheney, E., Buis, S., Launay, M., Constantin, J., Mary, B., Garc a de Cort zar-Atauri, I., Ripoche, D., Beaudoin N., Ruget, F., Andrianarisoa, K.S., Le Bas, C., Justes, E., L onard, J., 2015. Accuracy, robustness and behavior of the STICS soil-crop model for plant, water and nitrogen outputs: Evaluation over a wide range of agro-environmental conditions in France. *Environ. Model. Softw.* 64, 177-190.
- Dubus, I.G., Brown, C.D., Beulke, S., 2003. Sensitivity analyses for four pesticide leaching models. *Pest Manage. Sci.* 59, 962-982.
- FAO, 2014. World Reference Base for Soil Resources 2014 International Soil Classification System for Naming Soils and Creating Legends for Soil Maps. FAO, Rome.
- Flury, M., 1996. Experimental evidence of transport of pesticides through field soils-A review. *J. Environ. Qual.* 25, 25-45.

- FOCUS, 2000. "FOCUS groundwater scenarios in the EU review of active substances". Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference Sanco/321/2000 rev.2, 202 pp.
- Hossard, L., Archer, D.W., Bertrand, M., Colnenne-David, C., Debaeke, P., Ernfors, M., Jeuffroy, M.H., Munier-Jolain, N., Nilsson, C., Sanford, G.R., Snapp, S.S., Jensen, E.S., Makowski, D., 2016. A meta-analysis of maize and wheat yields in low-inputs vs conventional organic systems. *Agron. J.* 108, 1155-1167.
- Jordán, A., Zavala, L.M., Gil, J., 2010. Effects of mulching on soil physical properties and runoff under semi-arid conditions in southern Spain. *Catena* 81, 77-85.
- Larsbo, M., Roulter, S., Stenemo, F., Kasteel, R., Jarvis, N., 2005. An improved dual-permeability model of water flow and solute transport in the vadose zone. *Vadose Zone J.* 4, 398-406.
- Lammoglia, S.K., Moeys, J., Barriuso, E., Larsbo, M., Marín-Benito, J.M., Justes, E., Alletto, L., Ubertosi, M., Nicolardot, B., Munier-Jolain, N., Mamy, L., 2016. Sequential use of the STICS crop model and the MACRO pesticide fate model to simulate pesticides leaching in cropping systems. *Environ. Sci. Pollut. Res.* (online, DOI 10.1007/s11356-016-6842-7).
- Lindahl, A.M., Kreuger, J., Stenström, J., Gärdenäs, A.I., Alavi, G., Roulter, S., Jarvis, N.J., 2005. Stochastic modeling of diffuse pesticide losses from a small agricultural catchment. *J. Environ. Qual.* 34, 1174-1185.
- Malone, R.W., Ahuja, L.R., Ma, L., Wauchope, R.D., Ma, Q., Rojas, K.W., 2004. Application of the Root Zone Water Quality Model (RZWQM) to pesticide fate and transport: an overview. *Pest Manage. Sci.* 60, 205-221.
- Marín-Benito, J.M., Pot, V., Alletto, L., Mamy, L., Bedos, C., Barriuso, E., Benoit, P., 2014. Comparison of three pesticide fate models with respect to the leaching of two herbicides under field conditions in an irrigated maize cropping system. *Sci. Tot. Environ.* 499, 533-545.
- Morris, M.D., 1991. Factorial sampling plans for preliminary computational experiments. *Technometrics* 33, 161-174.
- Mortensen, D.A., Bastiaans, L., Sattin, M., 2000. The role of ecology in the development of weed management systems: an outlook. *Weed Res.* 40, 49-62.
- Pascual, J.A., Hart, A.D.M., Saunders, P.J., McKay, H.V., Kilpatrick, J., Prosser, P., 1999. Agricultural methods to reduce the risk to birds from cereal seed treatments on fenlands in eastern England. I. Sowing depth manipulation. *Agric. Ecosyst. Environ.* 72, 59-73.

- Pommel, B., Mouraux, D., Cappellen, O., Ledent, J.F., 2002. Influence of delayed emergence and canopy skips on the growth and development of maize plants: a plant scale approach with CERES-Maize. *Eur. J. Agron.* 16, 263-277.
- Queyrel, W., Habets, F., Blanchoud, H., Ripoche, D., Launay, M., 2016. Pesticide fate modeling in soils with the crop model STICS: Feasibility for assessment of agricultural practices. *Sci. Tot. Environ.* 542, 787-802.
- R Development Core Team, 2016. <https://www.r-project.org/> (accessed 20.05.16).
- Regulation EC No 1107/2009, 2009. Regulation of the European parliament and of the council of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC. *Off. J. Eur. Union*, L309.
- Ripoche-Wachter, D., Cufi, J., 2013. Stics, Version JavaStics 1.x / Stics v8.x (old name ModuloSTICS 1.2), User Guide, October 2013, 130 p.
- Ruget, F., Brisson, N., Delécolle, R., Faivre, R., 2002. Sensitivity analysis of a crop simulation model, STICS, in order to choose the main parameters to be estimated. *Agronomie* 22, 133-158.
- Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., Tarantola, S., 2008. *Global Sensitivity Analysis: the Primer*, John Wiley and Sons Ltd, Chichester.
- Scopel, E., Da Silva, F.A.M., Corbeels, M., Affholder, F., Maraux, F., 2004. Modelling crop residue mulching effects on water use and production of maize under semi-arid and humid tropical conditions. *Agronomie* 24, 383-395.
- Scopel, E., Triomphe, B., Affholder, F., Macena Da Silva, F.A., Corbeels, M., Valadares Xavier, J.H., Lahmar, R., Recous, S., Bernoux, M., Blanchart, E., de Carvalho Mendes, I., de Tourdonnet, S., 2013. Conservation agriculture cropping systems in temperate and tropical conditions, performances and impacts. A review. *Agron. Sustain. Dev.* 33, 113-130.
- Shipitalo, M.J., Malone, R.W., Ma, L., Nolan, B.T., Kanwar, R.S., Shaner, D.L., Pederson, C.H., 2016. Corn stover harvest increases herbicide movement to subsurface drains - Root Zone Water Quality Model simulations. *Pest Manage. Sci.* 72, 1124-1132.
- Soane, B.D., Ball, B.C., Arvidsson, J., Basch, G., Moreno, F., Roger-Estrade, J., 2012. No-till in northern, western and south-western Europe: A review of problems and opportunities for crop production and the environment. *Soil Till. Res.* 118, 66-87.
- Spink, J.H., Semere, T., Sparkes, D.L., Whaley, J.M., Foulkes, M.J., Clare, R.W., Scott, R.K., 2000. Effect of sowing date on the optimum plant density of winter wheat. *Ann. Appl. Biol.* 137, 179-188.

- Steffens, K., Jarvis, N., Lewan, E., Lindström, B., Kreuger, J., Kjellström, E., Moeys, J., 2015. Direct and indirect effects of climate change on herbicide leaching - A regional scale assessment in Sweden. *Sci. Tot. Environ.* 514, 239-249.
- Van Genuchten, M.T., Leij, F.J., Yates, S.R., 1991. The RETC code for quantifying hydraulic functions of unsaturated soils. Technical Report IAG-DW 12933934, US Salinity Laboratory, US Department of Agriculture, Agricultural Research Service, Riverside, CA.
- Vanuytrecht, E., Raes, D., Willems, P., 2014. Global sensitivity analysis of yield output from the water productivity model. *Environ. Model. Soft.* 51, 323-332.
- Vetsch, J.A., Randall, G.W., 2002. Corn production as affected by tillage system and starter fertilizer. *Agron. J.* 94, 532-540.