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Abstract

The current challenge in sustainable agriculture is to introduce new cropping systems to reduce pesticides use in order to reduce ground- and surface-water contamination. However, it is difficult to carry out in situ experiments to assess the environmental impacts of pesticides use for all possible combinations of climate, crop and soils, therefore *in silico* tools are necessary. The objective of this work was to assess pesticides leaching in cropping systems coupling the performances of a crop model (STICS) and of a pesticide fate model (MACRO). STICS-MACRO has the advantage of being able to simulate pesticides fate in complex cropping systems and to consider some agricultural practices such as fertilization, mulch or crop residues management, which cannot be accounted for with MACRO. The performance of STICS-MACRO was tested, without calibration, from measurements done in two French experimental sites with contrasted soil and climate properties. The prediction of water percolation and pesticides concentrations with STICS-MACRO was satisfactory, but it varied with the pedoclimatic context. The performance of STICS-MACRO was shown to be similar or better than that of MACRO. The improvement of the simulation of crop growth allowed better estimate of crop transpiration therefore of water balance. It also allowed better estimate of pesticide interception by the crop which was found to be crucial for the prediction of pesticides concentrations in water. STICS-MACRO is a new promising tool to improve the assessment of the environmental risks of pesticides used in cropping systems.

Keywords Modelling · Cropping systems · Pesticides · Agricultural practices · MACRO · STICS

Introduction

In line with European regulation (Directive 2009/128/EC), there is a need for a reduction of pesticide usage in order to reduce non-point contaminations, especially to ground- and surface-water, while maintaining the yields and quality of agricultural productions (Butault et al. 2010). This objective requires to change the production system and to design and introduce new innovative cropping systems which decrease the needs for chemical protection and mitigate the risks of water contamination (Mortensen et al. 2000).

A large number of new cropping systems can be designed combining various agronomical techniques such as those from IPM (Integrated Pest Management) or conservation agriculture (Aubertot et al. 2005; Lichtfouse et al. 2009; Ricci et al. 2011). The diversity of possible combinations makes it difficult to carry out *in situ* experiments that would be required to study the sustainability of each new system. A significant constraint in estimating the risk of detrimental environmental effects of pesticides used in these cropping systems is the large

variation in agricultural practices, soils, and climates that have a strong influence on the fate of pesticides (Mottes et al. 2014).

Therefore, *ex-ante* evaluation tools that are able to represent and to assess numerous options and to identify alternative systems were developed (Meynard 2008). These tools, based on multi-criteria decision-aid approach, can be used to qualitatively assess economic, social and environmental sustainability of production systems at the field scale. They provide the opportunity to assess a high number of innovative options across a large range of situations (e.g. Bockstaller et al. 2009; Bohanec et al. 2008; Dogliotti et al. 2004; Sadok et al. 2009). However they do not take into account direct and indirect effects of climate, pesticide and soil characteristics and they do not allow the assessment of pesticide flows and concentrations in the environment (soil, water, air).

One efficient way of assessing pesticides environmental impacts, i.e. their transfer to water, soil, and atmosphere, is to use process-based numerical models such as pesticides fate models (Vanclooster et al. 2000). Several models exist which account for the effects of both pedologic and climatic conditions on the transfer of each considered pesticide, however the representation of agricultural practices (tillage, organic matter management, mulch…) remains incomplete (Mottes et al. 2014). Recently, to better integrate crop management and crop growth in the simulation of agricultural pollutions, Queyrel et al. (2016) introduced a simplified pesticide fate module in the STICS crop model (Brisson et al. 1998). STICS can simulate the growth of a large range of crops under different agricultural practices (rotation, mixed crops, management residues, tillage…) and different soil and climatic conditions (Coucheney et al. 2015). The resulting STICS-Pest model therefore allowed to consider the diversity of agricultural practices. It was found to be as efficient as capacity pesticide fate models to predict pesticides leaching in some contexts. However, as underlined by the authors, some of the limits of STICS-Pest is the simplified formalism for water transfer, and the absence of non-linear sorption which 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). To address this problem, another innovative strategy is to combine the use of a pesticide fate model and of a crop model.

Among the pesticide fate models, MACRO (Larsbo et al. 2005) simulates water and pesticides flows in both soil micropores and macropores, and its performance is known to be good to predict the fate of pesticides under conventional crop management (e.g. Marín-Benito et al. 2014). In addition, MACRO is one of the models used in Europe for the assessment of pesticides leaching within the scope of their registration (FOCUS, 2000). However, although water and pesticides flows are rigorously described in MACRO, the description of the crop is maybe too simple as it only considers the maximum leaf area index (LAI), the maximum rooting depth and the

maximum crop height. Thus, the combination of MACRO and of a crop model such as STICS can be used to test whether a better modelling of crop growth can improve simulation of pesticides leaching for a wide variety of crop and management practices.

Therefore, the objectives of this work were (1) to develop a new modeling approach to assess pesticides leaching in cropping systems, based on a sequential use of the STICS model (to estimate variables such as the crop evapotranspiration) and of the MACRO model (forced with those variables as inputs), and (2) to test the performance of the STICS-MACRO resulting model, without calibration, by comparing its results to those provided by MACRO, parameterized for similar conditions, and then to compare the outputs of both models with measurements of pesticides concentrations in groundwater done in two French experimental sites.

Materials and methods

Models

MACRO pesticide fate model 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 between 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. The later is represented by a kinematic wave equation, with two hydraulic parameters: (1) the saturated hydraulic conductivity of macropores, and (2) an exponent reflecting macropores tortuosity and connectivity and how the conductivity increases with the degree of saturation. The water retention is described by a modified form of the van Genuchten function. Water exchange between micropores and macropores is considered as an instantaneous "discharge" when the matrix becomes over-saturated, while exchange in the other direction is modelled as a diffusive process controlled by an effective diffusion pathlength, as a surrogate parameter for the geometry of soil structure (Gerke and van Genuchten 1996). 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. While root depth and crop height are assumed to increase linearly until the crop reaches its maximum development, the increase of the LAI is divided in two phases, a slow linear growth phase (for describing autumn crop overwintering) and a fast non-linear growth phase until the LAI reaches its full extent. When the maximal development is reached, root depth, crop height and total LAI are kept constant until harvest, but the green LAI decreases (non-linearly) until the harvest date (where it reaches the "LAI

at harvest", another model parameter). Overall, the crop description is quite flexible, but it does not allow any physiological or climatic feedback-effect on the crop development: the crop growth is fully defined by the user and independent of other processes. Potential evapotranspiration can be calculated with the Penmann-Monteith equation, as a function of climate variables (minimum and maximum air temperature, wind speed, solar radiation and vapor pressure) and crop development characteristics (crop height and LAI) at each time step. Potential evapotranspiration can also be provided as an input variable (along with minimum and maximum air temperature). The actual plant transpiration is limited by water availability in each soil layer. The MACRO model also includes a mechanism of compensatory root water uptake that partly balance the effect of water availability. An important difference between STICS and MACRO is the description of soil evaporation. The latter calculates transpiration at the soil surface as a function of soil matric potential and bounded by the atmospheric demand. Below the soil surface, the effect of soil evaporation is simply driven by gradients in soil hydraulic head (Richards equation). Rainfall can be provided as input variable at a daily or an hourly time step. When the rainfall is provided at a daily time step, it is internally disaggregated at an hourly time step (at which the model runs). Pesticide dynamic can be very sensitive to the rainfall time step (and to the disaggregation parameter: the average rainfall intensity), especially when the soil is susceptible to macropore flow.

We used for this work a development version of the MACRO model (aiming at replacing the official release MACRO 5.2 in the future). For this work, the MACRO model was modified to use variable crop characteristics (green and total LAI, crop height and root depth) as forcing. The profile of root density is calculated internally in MACRO from the maximum root depth (and a shape parameter), both when the root depth is calculated internally and when supplied as forcing.

STICS crop model STICS (Simulateur mulTI disciplinaire pour les Cultures Standards) is a generic and dynamic crop model, with a daily time step, able to simulate the growth and yield of various crops but also the carbon, water and nitrogen balances of the soil-crop system by taking into account the effects of climate, soil, crop, and management practices (e.g. nutrient and organic fertilization, irrigation, soil tillage, and residues management) (Brisson et al. 1998). The crop is characterized by its aboveground biomass (carbon and nitrogen), LAI, as well as the number and biomass (carbon and nitrogen) of harvested crop organs. It follows that vegetative organs (leaves, ramifications or stems) are viewed as a whole. The plant's carbon metabolism drives crop growth with solar radiation intercepted by the canopy converted into shoot biomass. Crop development is driven by the accumulation

of degree days. The model simulates the behaviour of an average plant (i.e. not accounting for within field variability).

The soil is divided into five horizons, and each horizon is characterized by its bulk density, and by water contents at field capacity and at wilting point. Water transport in the soil is calculated daily for each 1-cm layer using a capacity approach. Plant roots, which enable the interactions between the soil and the crop, are defined with their length distribution in the soil profile. STICS responds to management practices by determining stress indices depending on the water input from irrigation and nitrogen input from fertilization. These indices can reduce leaf growth, root growth and biomass accumulation under water- and nutrient-limited growing conditions.

To simulate a cropping system, STICS requires inputs such as the seeding date, depth and density, the date and rate of mineral and organic fertilization, the date and amount of irrigation, and the date and method of soil tillage. This includes a description of crop residues, and organic products ploughed under since the STICS model also accounts for the decomposition of crop residues. If measured data are not available, STICS is also able to compute irrigation and fertilizer amounts according to plant needs. STICS was parameterized and evaluated for many crops such as wheat, maize, oilseed rape, sunflower, soybean, flax, tomato, sorghum, lettuce crops, mustard, sugarbeet, barley, and potato (Brisson et al. 2003). It can predict more than 200 output 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. The 8.4 version of STICS was used in this work.

Sequential use of STICS and MACRO Dedicated R packages (R Development Core Team 2015) were developed to automate the forcing of MACRO inputs with some STICS output variables (Fig. 1). The packages allow to sequentially (1) import predefined STICS and MACRO parameterization sets (one for each model), (2) simulate the crop rotation 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) optionally re-estimate the fraction of the spayed pesticide intercepted by the crop (based on STICS total LAI when the pesticide is sprayed), (6) run the MACRO model (with adapted parameterization, crop shape variables and potential evapotranspiration; Fig. 1), and finally (7) import MACRO simulation results. It is possible to choose whether both crop shape variables and potential evapotranspiration are “forced”, or only one of the two. 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.

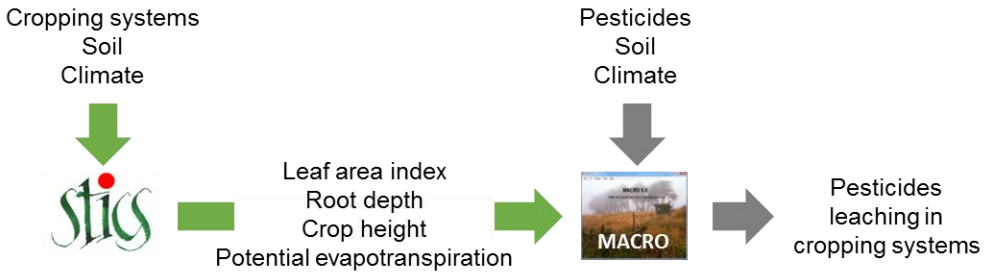

Fig. 1 Sequential use of STICS crop model and of MACRO pesticide fate model to simulate pesticides leaching in cropping systems

Because of the very different representation of crop growth and hydrological processes, the user needs to parameterize both models for the same site (climate and soil characteristics) before they can be run sequentially with the dedicated R routines.

Experimental sites

Two contrasting cropping systems in two French experimental sites located in Burgundy (Dijon-Epoisses) and Midi-Pyrénées (Lamothe) were selected for this study. They were chosen to reflect diversity in cropping practices, soils, crops, and climatic conditions.

Dijon-Epoisses The Dijon-Epoisses (47°20 N, 5°2 E) experimental site of INRA (referred as Dijon) was set up in 2000 to study the economic, social and environmental impacts of different innovative cropping systems (Chikowo et al. 2009). These systems combine several preventive methods against weeds (increased diversity of crop rotations, increased number of shallow tillage operations with mechanical weeding and false seed beds, choice of competitive cultivars). The soil is a clayey calcic Cambisol (FAO 2014) (Table 1). The site is divided in 5 plots of 1.7 ha each: there is one reference plot with an oilseed rape - winter wheat - winter barley rotation, and 4 plots where different innovative integrated weed management (IWM) cropping systems derived from the reference system are experimented. This work will focus on one of the IWM system using herbicides for weed control without mechanical weeding management. The crop sequence during the four simulated years was spring barley – winter oilseed rape – winter wheat – soybean (Table 2). Ploughing and other soil tillage operations were used when necessary for weed seed bank management. The straw residues of the previous crops were incorporated before sowing of the following crops. Some details of crop management for the 4 years are given in Table 2. The

simulation of pesticide leaching was focused on imazamox that was sprayed once, as Pulsar 40 formulation (BASF Agro SAS), the 1 July 2013 at 32 g ha^{-1}. This herbicide had never been applied on the plot before. The annual rainfalls were 829 mm in 2010, 692 mm in 2011, 788 in 2012, and 941 mm in 2013. The average annual temperature is 11°C with maximum and minimum mean monthly temperatures of 20°C and 2°C recorded in July and February, respectively.

Table 1 Dijon-Epoisses and Lamothe soils physicochemical and hydraulic characteristics. WILT: soil water content at wilting point; HCCF: soil water content at field capacity; TPORV: saturated water content, RESID: residual water content; ALPHA: alpha van Genuchten parameter; n: n van Genuchten parameter; KSATMIN: saturated hydraulic conductivity; CTEN: boundary (i.e. between macropores and micropores) soil water tension; KSM: boundary hydraulic conductivity; XMPOR: boundary water content; ASCALE: effective diffusion pathlength; ZN: tortuosity/pore size distribution factor

	Dijon-Epoisses			Lamothe[e]				
Depth (cm)	0-21	21-44	44-80	0-10	10-30	30-60	60-100	100-200
Clay (%)[a]	39.1	44.4	49.4	32.2	34.6	35.5	43.8	33.9
Silt (%)[a]	55.1	50.7	44.1	45.2	42.8	44.0	39.4	22.1
Sand (%)[a]	5.8	4.9	6.5	22.6	22.6	20.5	16.8	44
OC (%)[a]	1.86	1.14	0.63	1.38	1.07	0.95	0.71	0.24
pH (water)[a]	7.01	7.26	7.93	6.68	6.40	7.13	7.76	7.87
Bulk density (g cm^{-3})[a]	1.44	1.44	1.48	1.50	1.50	1.56	1.63	1.63
WILT (m^3 m^{-3})[a]	0.134	0.148	0.158	0.114	0.12	0.122	0.146	0.142
HCCF (m^3 m^{-3}) [b]	0.298	0.306	0.308	0.27	0.273	0.27	0.28	0.26
TPORV (m^3 m^{-3}) [b]	0.4588	0.505	0.456	0.414	0.419	0.406	0.399	0.381
XMPOR (m^3 m^{-3}) [b]	0.405	0.390	0.424	0.411	0.415	0.402	0.394	0.373
RESID (m^3 m^{-3}) [b]	0.092	0.102	0.095	0.08	0.083	0.081	0.084	0.071
ALPHA (cm^{-1}) [b]	0.01	0.0125	0.013	0.010	0.011	0.011	0.014	0.020
n (-)[b]	1.439	1.390	1.335	1.464	1.434	1.409	1.307	1.258
KSATMIN (m d^{-1}) [b]	0.064	0.139	0.050	0.528	1.560	0.24	0.024	0.024
KSM (m d^{-1}) [b]	0.001	0.004	0.017	0.014	0.024	0.034	0.007	0.026
CTEN (cm) [c]	40	40	50	10	10	10	10	10
ASCALE (mm) [d]	5	5	5	6	6	30	30	20
ZN (-) [c]	2	2	2	3	3	2	2	2

[a] Parameters that were directly measured in laboratory
[b] Estimated with RETC (RETention Curve) (Van Genuchten et al., 1991). For Dijon-Epoisses, parameters were determined from measured water retention curves fitted with RETC (Ugarte-Nano 2015; Ugarte-Nano et al. 2016)
[c] Estimated from Beulke et al. (2002)
[d] Estimated using MACRO 5.0/5.1 pedotransfer function
[e] For Lamothe, data are taken from Marín-Benito et al. (2014)

Table 2 Main crops characteristics of Dijon-Epoisses and Lamothe experimental sites used to parameterize STICS-MACRO and MACRO

		Dijon-Epoisses[a]	Lamothe[b]
2010	Crop	Barley	Bare soil
	Sowing / harvest dates	15 March 10 / 27 July 10	na
	Sowing density (kg ha^{-1})	150	na
	N rate (kg N ha^{-1})	110	na
	LAI (m^2 m^{-2}) at emergence / flowering / harvest	0.01 / 5 / 1	na
	Root depth at emergence / flowering (m)	0.01 / 1.1	na
	Crop height at emergence / flowering (m)	0.01 / 0.8	na
	Irrigation (mm)	0	na
2011	Crop	Oilseed rape	Maize
	Sowing / harvest dates	13 Sept. 10 / 12 July 11	18 April 11 / 14 Oct. 11
	Sowing density (kg ha^{-1})	3.5	27
	N rate (kg N ha^{-1})	158	160
	LAI (m^2 m^{-2}) at emergence / flowering / harvest	1[c] / 5 / 1	0 / 3.29 / 2
	Root depth at emergence / flowering (m)	0.2[c] / 1.1	0.01 / 0.8
	Crop height at emergence / flowering (m)	0.2[c] / 0.8	0 / 2.5
	Irrigation (mm)	0	250
2012	Crop	Winter wheat	Maize
	Sowing / harvest dates	24 Oct. 11 / 24 July 12	6 April 12 / 8 Oct. 12
	Sowing density (kg ha^{-1})	160	32.3
	N rate (kg N ha^{-1})	216	176
	LAI (m^2 m^{-2}) at emergence / flowering / harvest	1[c] / 5 / 1	0 / 3.29 / 2
	Root depth at emergence / flowering (m)	0.2[c] / 1.1	0.01 / 0.8
	Crop height at emergence / flowering (m)	0.2[c] / 0.8	0 / 2.5
	Irrigation (mm)	0	310
2013	Crop	Soybean	Maize
	Sowing / harvest dates	13 May 13 / 22 Oct. 13	23 April 13 / 9 Oct. 13
	Sowing density (kg ha^{-1})	120	35.3
	N rate (kg N ha^{-1})	0	96
	LAI (m^2 m^{-2}) at emergence / flowering / harvest	0.01 / 4 / 3	0 / 3.29 / 2
	Root depth at emergence / flowering (m)	0.01 / 0.8	0.01 / 0.8
	Crop height at emergence / flowering (m)	0.01 / 0.8	0 / 2.5
	Irrigation (mm)	40	205
2014	Crop	na	Maize
	Sowing / harvest dates	na	14 April 14 / 8 Oct. 14
	Sowing density (kg ha^{-1})	na	34.2
	N rate (kg N ha^{-1})	na	170
	LAI (m^2 m^{-2}) at emergence / flowering / harvest	na	0 / 3.29 / 2
	Root depth at emergence / flowering (m)	na	0.01 / 0.8
	Crop height at emergence / flowering (m)	na	0 / 2.5
	Irrigation (mm)	na	150

na: not applicable

[a] For Dijon-Epoisses, all data are measurements except LAI and root depth that were determined according to Jarvis et al. (2007)

[b] For Lamothe, all data are measurements except the leaf area index at harvest which was set to 2 according to Marín-Benito et al. (2014)

[c] For winter crop, MACRO needs the transition LAI, root depth and crop height when the crop switch from a slow to a fast growth

Lamothe The Lamothe (43°31 N, 3°51 E) experimental site of INP EI Purpan was set up in 2011. The objective was to develop and to evaluate the agronomic, environmental, and socio-economic performance of low input maize cropping systems. Four maize cropping systems differing in their input use intensity and representing a gradient from a high-input conventional monoculture to a low-input integrated cropping system rotation were designed and experimented. The site is divided into 2 blocks of 15 plots of 0.08 ha each (Alletto et al. 2015). The soil is a stagnic Luvisol (FAO 2014) with an illuvial clay horizon between 35 and 60 cm (Table 1). The test of STICS-MACRO will be based on the reference high-input conventional maize system (Alletto et al. 2015; Marín-Benito et al. 2014). The main agricultural operations consisted of a conventional tillage with a spring mouldboard ploughing (25–28 cm depth). In winter, during the fallow period, no crop was grown (bare soil). Water and nitrogen were supplied as required to avoid any stress so as to reach the potential yields (Table 2). The dates of sowing and harvest are summarized in Table 2. Chemical control of weeds was following common practices for conventional maize production in the South-West of France. This study will focus on S-metolachlor, one of the most used herbicide in maize. S-metolachlor was sprayed once a year from 2011 to 2014 (it had never been applied before): 1.25 kg ha^{-1} (Mercantor Gold formulation, Syngenta Production France SAS) the 5 May 2011; 1.52 kg ha^{-1} (Calibra, Syngenta Production France SAS) the 3 May 2012; 1.34 kg ha^{-1} (Mercantor Gold) the 7 May 2013; and 1.52 kg ha^{-1} (Calibra) the 16 April 2014. The annual rainfalls were 636 mm in 2010, 466 mm in 2011, 581 mm in 2012, 799 mm in 2013, and 653 mm in 2014. The mean annual daily temperature is 13.5°C with maximum and minimum mean monthly temperatures of 21.4°C and 5.5°C recorded in August and February, respectively.

Measurements In both sites, the details of farming operations (dates and characteristics of tillage, sowing, pesticides spraying, and harvest), and crop grain yields were recorded. Water flows and herbicides leaching were monitored using two wick lysimeters installed at a depth of 0.5 m since 2012 in Dijon, and one tension plate lysimeter (with a fixed pressure at -100 hPa) installed at a depth of 1 m since 2011 in Lamothe. Leachates were periodically sampled and they were kept at 4°C in darkness until analysis. Pesticides analyses were done by the Laboratoire Départemental d'Analyses de la Drôme (Valence, France) accredited by COFRAC (French Committee of Accreditation). For both imazamox and S-metolachlor, the limit of quantification and the limit of detection were 0.02 µg L^{-1} and 0.007 µg L^{-1}, respectively.

Model parameterization

The models input parameters were mainly based on literature, pedotransfer functions or default values taken from the user's manuals, and on some measurements (soil characteristics, crops management). We chose to test the performances of the models using a simplified parameterization to be as close as possible to a risk assessment in an unsampled location, while still enabling some comparisons between measurements and simulations. Additionally, the possible bottom boundary conditions for MACRO and STICS do not allow a fully satisfactory representation and calibration of wick and tension plate lysimeters. For the Lamothe case study, soil, crop and S-metolachlor parameterization was based on uncalibrated values of Marín-Benito et al. (2014) (Tables 1, 2 and 3).

Table 3 Freundlich sorption coefficients (Kf) and half-lives (DT50) of imazamox in the Dijon-Epoisses soil profile and of S-metolachlor in the Lamothe soil profile. The Freundlich coefficients nf were 0.89 for imazamox and 1 for S-metolachlor in all soil layers.

Imazamox in Dijon-Epoisses soil			S-metolachlor in Lamothe soil		
Depth (cm)	Kf	DT50 (days)	Depth (cm)	Kf[d]	DT50 (days)[d]
0-21	0.34[a]	70[a]	0-10	0.8	29
21-30	0.21[b]	70[c]	10-30	0.62	29
30-44	0.21[b]	140[c]	30-60	0.55	58
44-60	0.11[b]	140[c]	60-100	0.41	99
60-80	0.11[b]	233[c]	100-200	0.14	0

[a] From PPDB (2016)
[b] Variation of Kf with depth was determined according to soil organic carbon content (Table 1)
[c] Variation of DT50 with depth was determined according to FOCUS (2000)
[d] From Marín-Benito et al. (2014)

Soils For the Dijon site, the soil characteristics such as sand, silt, clay, and organic carbon contents, bulk density and pH value were derived from field data (Table 1). The water contents at wilting point (WILT) and field capacity (HCCF), the water retention parameters (TPORV: saturated water content; XMPOR: boundary water content; RESID: residual water content), the saturated hydraulic conductivity (KSATMIN), the boundary hydraulic conductivity (KSM), and the van Genuchten's soil-water retention parameters (ALPHA, n) were determined from measured soil water retention curves (Ugarte-Nano 2015; Ugarte-Nano et al. 2016) fitted with RETC (RETention Curve) (Van Genuchten et al. 1991) (Table 1). The effective diffusion pathlength (ASCALE), which controls the exchange of both water and solute between the micropores and macropores, was estimated from the MACRO

5.0/5.1 pedotransfer function of the model. The tortuosity/pore size distribution factor for macropores (ZN), and the parameter which defines the boundary soil water pressure head between micropores and macropores (CTEN) were determined following the recommendations of Beulke et al. (2002) (Table 1). Soil inputs parameters for which measurements were not available were set to the default values indicated in STICS and MACRO user's manuals. For the Lamothe site, as indicated above, soil parameterization was done according to Marín-Benito et al. (2014) (Table 1). For both sites, the simulated soil profiles were divided into five horizons (Table 3) and 200 numerical layers. The soil bottom boundary condition in MACRO was set to unit hydraulic gradient.

Climate The climatic input data needed in STICS-MACRO and MACRO are daily rainfall, air temperature, global solar radiation, relative humidity and wind speed. For Dijon, the data were obtained from the INRA Epoisses meteorological station located close to the experimental site (Climatik, 2015). For Lamothe, the data were collected from the meteorological station located at the experimental site. In both cases, potential evapotranspiration was calculated with the Penman equation (Penman 1948).

Crops and agricultural practices To simulate crops development, STICS-MACRO required crops and cultivar parameters and detailed agricultural practices (sowing date and density, harvest time, fertilization, irrigation, tillage, mulch incorporation). These data were recorded for each site (Table 2), except the cultivar parameters which were available in STICS as default values (Brisson 2008). As indicated before, MACRO only needs maximum LAI, root depth and crop height to simulate crop growth (Table 2).

Pesticides Imazamox (2-[(RS)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl]-5-methoxymethylnicotinic acid) is a selective herbicide used for weed control in soybean and sunflower crops. It is an acid with a pKa of 2.3, having a low vapor pressure (0.0133 mPa) but a very high solubility in water (626 g L^{-1}) (PPDB 2016). S-metolachlor (mixture of 80-100% 2-chloro-N-(6-ethyl-o-tolyl)-N-[(1S)-2-methoxy-1-methylethyl]acetamide and 20-0% 2-chloro-N-(6-ethyl-o-tolyl)-N-[(1R)-2-methoxy-1-methylethyl]acetamide) is also a selective herbicide which is mainly used for pre- or post-emergence weed control in maize crop. It has a moderate vapor pressure (3.7 mPa) and a high solubility in water (0.48 g L^{-1}) (PPDB 2016). The main properties characterizing their fate in soils are summarized in Table 3. The variation in the degradation rates with depth was determined according to FOCUS (2000). Sorption was assumed to be proportional to the organic carbon content of the different horizons. The fraction of sorption sites attributed to the macropore (FRACMAC), as needed in MACRO, was set to 0.02 (Dubus

et al. 2003). Interceptions of 10% of imazamox by soybean crop, and of 2% of S-metolachlor by maize crop when applied post-emergence (Marín-Benito et al. 2014) were assumed to parameterize MACRO.

Simulations For Dijon, the simulation was carried out from 1st January 2009 to 31st December 2013, and for Lamothe, from 10th July 2010 to 31st December 2014. This allowed to add a warm-up period of at least 9 months before simulation of the first crop starts. In both cases, initial soil water content was set at field capacity, and an average soil mineral N content of 5 kg N ha^{-1} for each layer of 25 cm was used to initialize STICS.

Evaluation of models performance

The performance of STICS-MACRO and MACRO was assessed by studying their ability to simulate (1) crop growth, (2) water flows, and (3) pesticides leaching. Four outputs were thus selected for STICS-MACRO: the crop grain yield, the LAI, the amount of water percolated at the monitored depths (0.5 or 1 m), and the pesticides concentrations in the soil solution. For MACRO, the selected outputs were LAI, percolated water and pesticides concentrations. The performance of STICS-MACRO and MACRO was quantitatively assessed by calculating three statistical indices: the modeling efficiency (*EF*), the Pearson correlation coefficient (*r*), and the root mean square error (*RMSE*, expressed as a percentage) (Smith et al. 1996). These indices were calculated as follows:

$$EF = 1 - \frac{\sum_{i=1}^{n}(S_i - O_i)^2}{\sum_{i=1}^{n}(O_i - O_m)^2} \quad (1)$$

$$r = \frac{\sum_{i=1}^{n}(O_i - O_m)(S_i - S_m)}{\sqrt{\sum_{i=1}^{n}(O_i - O_m)^2} \times \sqrt{\sum_{i=1}^{n}(S_i - S_m)^2}} \quad (2)$$

$$RMSE = \frac{100}{O_m} \times \sqrt{\frac{1}{n}\sum_{i=1}^{n}(S_i - O_i)^2} \quad (3)$$

where S_i and O_i are the simulated and observed values, respectively, S_m and O_m are the mean of the simulated and observed values, respectively, and n is the number of sampling dates.

EF ranges from -∞ to 1, with *EF*=1 indicating a perfect match. If *r*=+1 (-1), then there is a perfect positive (negative) correlation between simulated and measured values; if *r*=0, then there is no linear correlation between simulations and measurements. The lower limit for *RMSE* is 0, in which case there is no difference between measured and simulated values.

Results and discussion

Performance of STICS-MACRO and MACRO in predicting crop growth

The simulated yields, using STICS (before the subsequent MACRO simulation), agreed well with the observed ones for all crops, both in Dijon and in Lamothe (Fig. 2), as shown by the very good values of the statistical indices: *EF*=0.90, *r*=0.91, and *RMSE*=13%. These results are as good as those obtained in previous studies where STICS was used to simulate yield and water balance without calibration and using default values (Constantin et al. 2015).

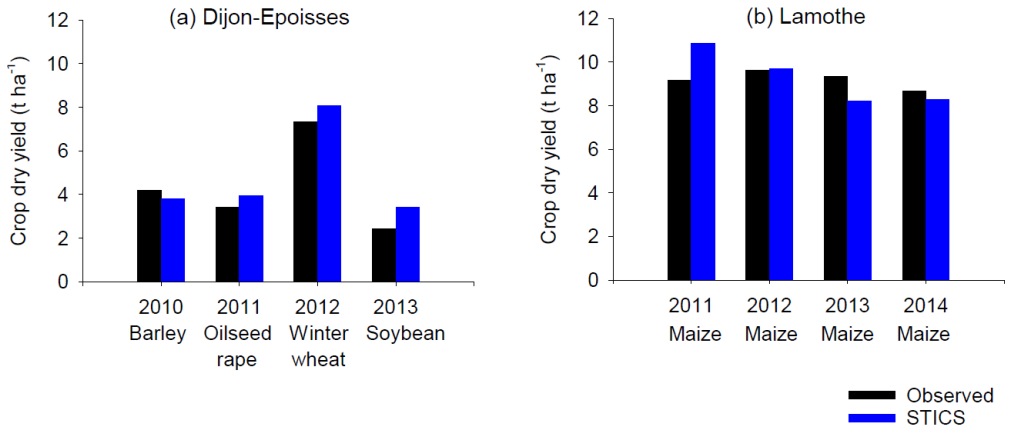

Fig. 2 Observed and simulated (with STICS) dry yields of barley, oilseed rape, winter wheat and soybean in Dijon-Epoisses (a), and of maize in Lamothe (b)

The LAI simulated by STICS and by MACRO are compared in Fig. 3. For the Dijon case study, the maximum LAI as predicted by STICS were equal to 2.6 for barley, 3.5 for oilseed rape, 5.6 for wheat, and 6.5 for soybean. STICS was able to distinguish the four crops while MACRO simulated the same maximum LAI (5.0) for barley, oilseed rape and winter wheat because of the way it has to be parameterized (see Materials and methods section) (Fig. 3a). In STICS, the crop growth depends on the interactions between crop, soil, climate and management practices that allow discrimination of crops and crop cycles. From experiments carried out in France, Lemaire et al. (2008) showed that high N fertilization application rate of 240-300 kg ha^{-1} per year increased the values of LAI of wheat until 6. As 216 kg N ha^{-1} were applied in 2012 at the Dijon site (Table 2), the predicted LAI of wheat agreed well with their results. The simulated LAI of oilseed rape was also consistent with that observed by Lemaire et al. (2008), being in average lower than 4 for N application rates of 160 kg ha^{-1} (Table 2). To the best of our knowledge, no LAI value has been published for barley in France. In dryer conditions in Spain, the LAI of barley was shown to be lower than 2 (Gabrielle et al. 2002), therefore the STICS LAI of 2.6 seems

acceptable. Finally, for soybean, STICS may have overestimated the maximum LAI as the simulated one was found to be 6.5 (Fig. 3a). Indeed, Jégo et al. (2010) showed that the European soybean cultivars defined in STICS lead to a significant overestimation of LAI. For the maize monoculture as experimented in Lamothe, MACRO simulated the same variation of LAI over the four years, independently of the climatic conditions or fertilizer use, while STICS predicted different evolutions of LAI (Fig. 3b). From 2011 to 2014, STICS simulated an average maize maximum LAI of about 3.8, the highest being 4.3 in 2011. This value is a bit higher than the measured LAI of 3.29 (Marín-Benito et al., 2014), but is consistent with the value obtained by Alletto et al. (2015) who used STICS to simulate the maize growth in Lamothe, and also obtained a maximum LAI of 4.3. The differences in the simulations of LAI have an effect on the simulated cumulated evapotranspiration which will have an impact on the water balance (Table 4).

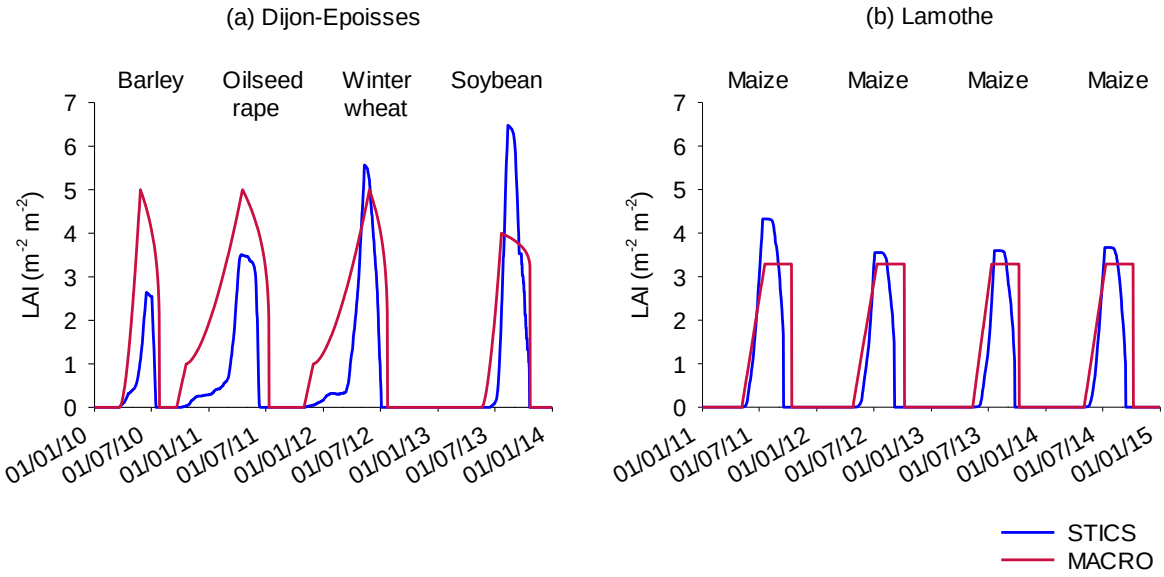

Fig. 3 Comparison of LAI simulated by STICS and by MACRO in Dijon-Epoisses (a) and Lamothe (b) experimental sites

Table 4 Soil water balance simulated by STICS-MACRO and MACRO. Soil profile is at 0.8 m depth at Dijon-Epoisses and at 2 m depth at Lamothe. The water balance is showed from 1st January 2009 to 31st December 2013 in Dijon-Epoisses, and from 10th July 2010 to 31st December 2014 in Lamothe.

	Dijon-Epoisses		Lamothe	
	STICS-MACRO	MACRO	STICS-MACRO	MACRO
Precipitation + Irrigation (mm)	4341	4341	4059	4059
Actual evapotranspiration (mm)	2535	2332	2575	3134
Seepage at bottom of profile (mm)	1779	1981	1368	877
Surface runoff (mm)	43	45	27	12
Change in soil water storage in the soil profile (mm)	+16	+17	-89	-36

As a summary, STICS was demonstrated to be good to capture differences in phenology among the crops and to capture how the crop growth is affected by changes in the environmental conditions (especially climatic conditions).

Performances of STICS-MACRO and MACRO in predicting water percolation

The total water balance simulated by MACRO and STICS-MACRO is shown in Table 4. For Dijon, the cumulative rainfall and irrigation from 1st January 2009 to 31st December 2013 was 4341 mm. Despite both models used the same climatic data, STICS-MACRO calculated 9% more evapotranspiration than MACRO (Table 4). These differences led to smaller simulated water drainage at the bottom of the soil profile with STICS-MACRO than with MACRO. For Lamothe, the cumulative rainfall and irrigation was 4059 mm from 10th July 2010 to 31st December 2014. Unlike Dijon, STICS-MACRO calculated 22% less evapotranspiration than MACRO and thus higher amount of water at the bottom of the soil profile (Table 4).

In the Dijon experimental site, one of the two wick lysimeters was flooded at several sampling dates because of groundwater table rise, therefore complete dynamic of water measurement was only exploitable for one of the lysimeters. The total amount of measured percolated water in this lysimeter was 190 mm (Fig. 4a). The corresponding simulated amounts of water were consistent with the observed value: 171 mm for STICS-MACRO and 174 mm for MACRO (Fig. 4a). For Lamothe, 215 mm of water were detected in the tension plate lysimeter

over the whole period of measurement (Fig. 4b). In this site, the tension plate lysimeter only collected water at soil pressure head higher than -100 hPa. Therefore, daily water percolation as simulated by MACRO and STICS-MACRO at 1 m depth was considered or not depending on the daily pressure head at the same depth: in models outputs, we discarded (set to 0) any water percolation occurring when the soil pressure head was lower than -100 hPa (Marín-Benito et al. 2014). STICS-MACRO simulated a cumulated amount of percolated water of 282 mm which resulted in an overestimation of 24%, but on the contrary, MACRO only simulated 86 mm leading to an underestimation of 60% of the observed amount (Fig. 4b). The low amount of percolated water as simulated with MACRO is mainly due to the high simulated evapotranspiration compared to STICS-MACRO (Table 4). This is consistent with the results of Giannouli and Antonopoulous (2015) and Marín-Benito et al. (2014) who showed that MACRO tends to simulate higher evapotranspiration than other models.

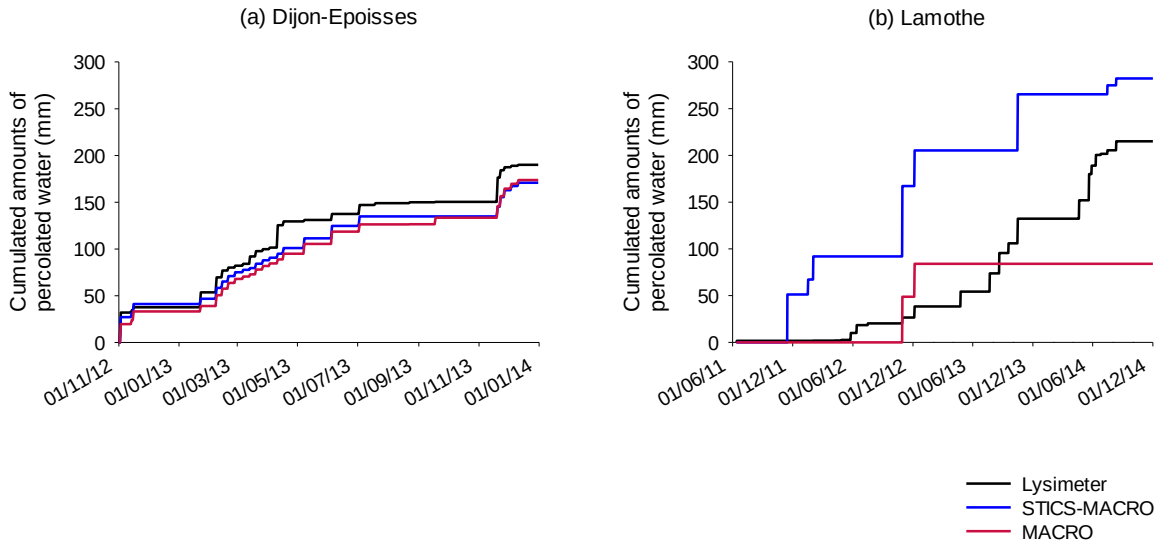

Fig. 4 Observed (in lysimeters) and simulated (with STICS-MACRO and MACRO) cumulated water percolation in Dijon-Epoisses (a) and Lamothe (b) experimental sites

The performance of both STICS-MACRO and MACRO to simulate water percolation was good for Dijon but poor for Lamothe (Fig. 4 and 5, and Table 5). This variability of the response of the models among different sites was also observed in many studies (e.g. Moeys et al. 2012; Queyrel et al. 2016). In general, the dynamics of the two models showed similar trends (Fig. 5a and b) but STICS-MACRO performed better than MACRO because of a better description of crop development which has a strong impact on water balance through transpiration (Table 4).

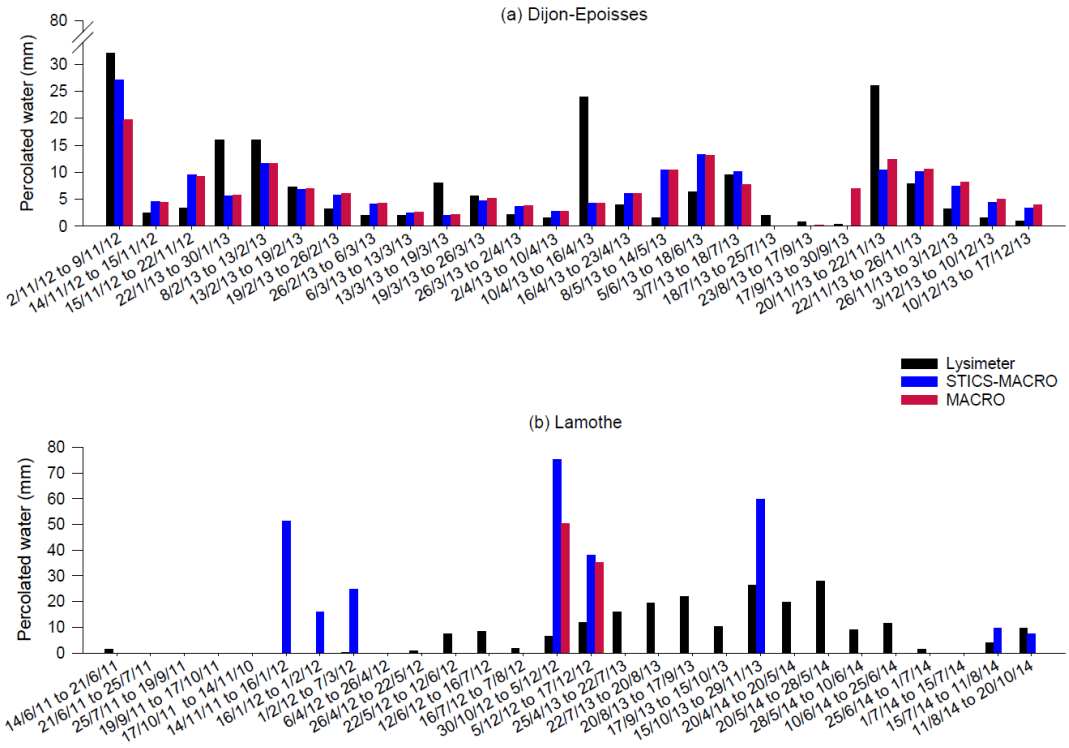

Fig. 5 Observed (in lysimeters) and simulated (with STICS-MACRO and MACRO) water percolation in Dijon-Epoisses (a) and Lamothe (b) experimental sites

Table 5 Goodness-of-fit statistics for STICS-MACRO and MACRO predictions of water percolation and pesticides leaching in Dijon-Epoisses and Lamothe experimental sites (EF: modeling efficiency; r: correlation coefficient; RMSE: root mean square error)

	Dijon-Epoisses		Lamothe	
	STICS-MACRO	MACRO	STICS-MACRO	MACRO
Water percolation				
EF	0.42	0.35	-5.22	-1.9
r	0.66	0.61	0.09	0.03
RMSE (%)	87	92	279	191
Pesticide leaching				
EF	-1.00	-1.19	-0.18	-0.21
R	-0.52	-0.58	0.13	-0.14
RMSE (%)	175	214	236	>1000

For Dijon, none of the models was able to reproduce the peaks of water percolation of April and October 2013 which correspond to heavy rain events: 24 mm of rain from 10 to 16 April, and 25.5 mm of rain from 19 to 22 November with a rain event of 18.5 mm on 19 November. Several hypotheses could explain the underestimation of water transfer by the models: (1) the lateral flows above or just below the lysimeter are not simulated by the one-dimensional models (Marín-Benito et al., 2014); (2) the lysimeters may capture more water than expected especially when initial conditions are humid (Cattan et al. 2007; Louie et al. 2000); (3) in MACRO, the daily rainfall data are converted into hourly rainfall data, and the default average rainfall intensity (2 mm h^{-1}) may be inappropriate, as intense rainfall events are more likely to generate preferential flow (McGrath et al. 2009; Moeys et al. 2012); (4) wick and tension plate lysimeters will start percolating at a lower tension (less saturated) than in a free drainage lysimeter as simulated by MACRO, where water percolates only when soil is almost saturated, and thus the former will collect more water. However, apart from these two events, the performance of STICS-MACRO and MACRO to simulate the water dynamic was good (Fig. 4a and 5a, and Table 5).

For Lamothe, none of the models was able to simulate the water dynamic, and the statistical indices were poor (Fig. 5b and Table 5). MACRO only simulated two events of water percolation, both in December 2012, but it did not simulate any other percolation over the observation period. The two December events were overestimated by MACRO by a factor 8 and 3, respectively. As indicated before, this can be due to the fact that MACRO simulates a free drainage lysimeter. STICS-MACRO simulated more events of water percolation than MACRO but it also overestimated the percolated amounts, except in October 2014 (Fig. 5b). It has to be noted that STICS-MACRO predicted correctly the percolation of water in August and October 2014 at the end of the experiment. Despite it considerably underestimated the observed water percolation, MACRO got the best performance in terms of RMSE and EF, but STICS-MACRO showed the better value of r (Table 5). The lack of good representation of water percolation could also be due to the fact that the soil hydraulic properties are constant in MACRO, however they vary with time and space as observed by Ugarte-Nano et al. (2015) in Dijon and by Alletto et al. (2015) in Lamothe.

The performance of STICS-MACRO to predict water percolation was found to be good and better than that of MACRO for the Dijon case study but poor and as poor as that of MACRO for the Lamothe case study. The detailed description of the crop development in STICS-MACRO is expected to allow better estimate of transpiration and therefore better estimate of water balance. It must be reminded that the models were used without calibration to test their potential for generic use.

Performances of STICS-MACRO and MACRO in predicting pesticides leaching

Observed and simulated imazamox concentrations measured in the Dijon lysimeter are compared in Fig. 6a. Imazamox was observed few days after its application, which was done on the 1 July 2013, and the concentration was high: 0.852 µg L^{-1}. Indeed, there was a strong rainfall event on the 2 July 2013 (18 mm) that can explain the rapid leaching of imazamox. This rapid transfer also indicates that it was probably due to preferential flows. Imazamox was then detected two times in November at 0.151 and 0.338 µg L^{-1}, before its concentrations decreased below the limit of detection (Fig. 6a). Over the second long time period of sampling, from 22 August to 17 December 2013, imazamox was also observed at a high concentration of 0.267 µg L^{-1} (Fig. 6a). These results are consistent with its low sorption coefficient (Table 3) and with other observations (Cessna et al. 2012). Both models failed to reproduce the first occurrence of imazamox following its application (Fig. 6a). Indeed, the low performance of pesticide fate models to reproduce early concentrations of pesticides following their application was frequently observed (e.g. Brown et al. 2004; Marín-Benito et al. 2014). As indicated by Brown et al. (2004), macropore flow is a highly stochastic process and it is thus difficult to simulate detailed behaviour over single events with great accuracy. STICS-MACRO and MACRO showed the same trend with a gradual increase in the concentrations of imazamox, and with an overestimation of the latest concentrations from 26 November to 10 December 2013 (Fig. 6a). In addition, MACRO overestimated the concentrations observed from 17 October to 26 November 2013 contrary to STICS-MACRO which simulated values very close to the observed ones (Fig. 6a). Finally, both models simulated well the concentrations of imazamox in the pooled sample from 22 August to 17 December 2013, but MACRO was closer to the observed value than STICS-MACRO (Fig. 6a). This could indicate that models performed better to simulate average concentration over long time period than the dynamic of concentrations on short time periods. Nevertheless, STICS-MACRO seemed to better capture the short time period dynamic of imazamox leaching than MACRO. In general, the simulated concentrations were in the same order of magnitude as observations, but because of the underestimation of the first peak of imazamox and of the overestimation of the two last observations, the goodness-of-fit statistics were poor (Table 5). Additional simulations showed that the overestimation of imazamox concentration with MACRO was due to an underestimation of the pesticide interception by the crop canopy, which is corrected when MACRO is forced with the LAI calculated by STICS in STICS-MACRO. Therefore, a manual calibration of the interception allowed to strongly improve the results of MACRO (data not shown). This highlights the importance of a good simulation of crop growth as a function of climatic and agronomic conditions to better estimate pesticide interception and therefore better estimate the concentrations of pesticides in water.

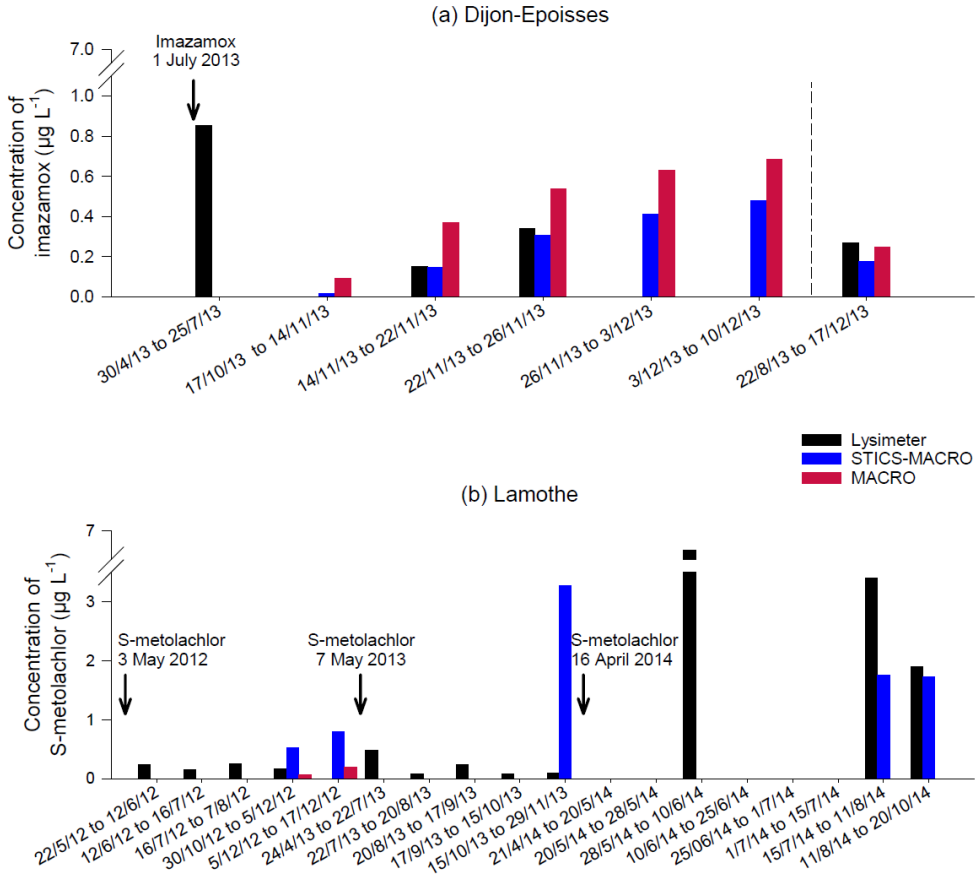

Fig. 6 Observed (in lysimeters) and simulated (with STICS-MACRO and MACRO) imazamox concentrations in Dijon-Epoisses (a) and S-metolachlor concentrations in Lamothe (b). The arrows indicate the dates of herbicides applications

S-metolachlor was always detected in Lamothe lysimeter in 2012 and 2013 with concentrations ranging from 0.08 to 0.48 µg L^{-1}. On the contrary, it was only detected three times in 2014 but at very high concentrations: from 1.9 to 6.66 µg L^{-1} (Fig. 6b). In any case, the observed S-metolachor concentrations were higher than the 0.1 µg L^{-1} regulatory limit (Directive 98/83 EC) which is consistent with the low value of its sorption coefficient (Table 3), and with several observations (e.g. Milan et al. 2015). As for water percolation, the simulation of pesticide leaching in Lamothe was poor (Fig. 6b, and Table 5). In particular, one peak of S-metolachlor observed from 29 May to 10 June 2014 (6.66 µg L^{-1}) was not simulated by both models (Fig. 6b). This peak corresponded to strong rain events happened on 25 and 26 May (12 and 14 mm, respectively) combined with one irrigation episode of 30 mm the 5 June. From 16 July to 11 August 2014, four major rain events (28, 22, 20 and 13 mm) and two irrigation episodes of 30 mm each could explain the leaching of S-metolachlor at a high concentration of 3.4 µg L^{-1} (Fig. 6b). The uncalibrated MACRO parameterization was not able to reproduce this concentration but

STICS-MACRO simulated a concentration of 1.75 µg L^{-1} equal to half of the observed concentration. The concentration of S-metolachor observed from 12 August to 20 October 2014 also corresponds to several rain events ranging from 15 to 20 mm. It was well predicted by STICS-MACRO but not by MACRO (Fig. 6b). MACRO failed to reproduce the concentrations of S-metolachlor probably because it simulated high evapotranspiration compared to STICS-MACRO which led to lower amount of percolated water (Table 4). As for imazamox in Dijon, the goodness-of-fit statistics were poor (Table 5) but they were higher for STICS-MACRO than for MACRO. STICS-MACRO matched the observations at 9 sampling dates over 18 sampling dates, i.e. it simulated either pesticide absence in water when the concentrations in the lysimeter were lower than the pesticide detection limit or it was able to simulate the presence of the pesticide when it was detected, while MACRO matched observations at only 6 sampling dates over the 18. The poor performance of both models in simulating S-metolachlor concentrations in Lamothe may be due to their difficulty to simulate water flows. However, the work of Moeys et al. (2012) suggests that improving the estimation of solute transport parameters is probably more important than the estimation of water flow parameters.

The sequential use of STICS and MACRO allowed to combine a good representation of the crop through STICS and a good representation of water and pesticides leaching in soils through MACRO as water transfer in STICS is not accurate enough (Queyrel et al. 2016). As underlined by Jacobsen et al. (2008), considering uncertainty related to (1) converting soil physical data to soil hydraulic properties by curve fitting or pedotransfer functions, (2) what extend locally measured samples represent the spatial scale of interest, (3) the ability of the model to capture major controls of leaching, and (4) the absence of calibration, then differences between observed and simulated concentrations by up to one order of magnitude at most may not be so significant. Therefore, STICS-MACRO was found efficient to simulate pesticide concentration and offer the advantage to allow parameterization of complex agricultural systems and to simulate the crop growth as a function of climate, soil and agricultural practices (fertilization, irrigation…).

Conclusion

The objective of this work was to develop a new tool based on the sequential use of the STICS model and of the MACRO model to assess pesticides leaching in cropping systems. STICS-MACRO was tested from measurements of the concentrations of two herbicides having similar physico-chemical properties, imazamox and S-metolachlor, in two different soil and climate contexts. The results were also compared to simulations done with MACRO. Both models were parameterized using pedotransfer functions, guidance documents and literature, and no calibration

was done. In this stringent conditions, the performance of STICS-MACRO to simulate water percolation and pesticides concentrations was acceptable, but it depended on the pedoclimatic context, and it was similar or better than that of MACRO. The improvement of the simulation of crop growth allowed better estimate of crop transpiration therefore of water balance. It also allowed better estimate of pesticide interception by the crop which was found to be crucial for the prediction of pesticides concentrations in water. STICS-MACRO is a credible alternative to improve MACRO to study agronomic practices scenarios avoiding prior calibration phase. It offers the advantage of being able to simulate complex cropping systems and to consider some agricultural practices such as fertilization, mulch, crop residues management, etc. Further tests are needed to ensure STICS-MACRO can be used to assess pesticides flows in a large range of situations. In particular, agro-pedoclimatic conditions involving sandy or heavy clay soils, cold and warm climates, and various crops and cropping systems have to be studied. These conditions will consequently allow the test of different pesticides (for example, pesticides more sorbed and more persistent than imazamox and S-metolachlor). Tests are also needed on long term time series as it is usually done for probabilistic risk assessment. However the STICS-MACRO modelling approach is promising to improve the assessment of the environmental risks of pesticides used in cropping systems.

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