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Pesticide transfer models in crop and watershed systems: a review

Charles Mottes · Magalie Lesueur-Jannoyer ·
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Abstract Pesticides are now occurring worldwide in almost all water resources, thus threatening the health of humans and other life. As a consequence, there is a strong social demand for designing safe cropping systems with less or no hazardous pesticides. Safe cropping systems can be designed now using pesticide transfer models. These models are mathematical tools that allow to predict the flow and concentration of pesticides in a field or a watershed. Here, we review the effects of agricultural practices on runoff, leaching, erosion, and drift from eight watershed models and nine field models. Our main findings are the following: (1) though models claim they account for practices, their effects cannot be represented. We present a method and four practice levels to assess the effects of practices in models, using tillage as an example. (2) The conceptual structure of the model highly influences the predicted distribution and transfer of pesticides. For instance, the pesticide levels remaining on the soil surface after plowing ranges from 0 % of the dose applied for the MIKE SHE–DAISY model to 100 % for GLEAMS, annAGNPS, SoilFug, and PestLCI. Only the Root Zone Water Quality Model (RZWQM) simulates pesticide interception by mulch during pesticide application. (3) Models should better take into account mulching, e.g., plastic, crop residues and associated crops, and other innovative practices. (4) A change in scale is needed for drift in watershed models. Here, topological watershed representations are the most

promising way for upscaling the effects of practices. (5) Non-conservative calculations of pesticide interception by watershed mitigation structures (SWAT) should be carefully checked because these calculations underestimate the risk of pollution at the outlet. How models simulate practices will no longer be a secret for model users who apply our methodology and recommendations when selecting a model. We provide recommendations for improving tools to assess practices.

Keywords Pesticides · Catchment · Watershed · Field · Agricultural practice · Best management practice · Mitigation practice · Model · Water pollution

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1 Introduction

In agriculture, the control of pests and weeds has always been a major problem worldwide. Since the 1930s–1940s, several families of chemical compounds have been synthesized to protect crops against pests and weeds while increasing yield and commercial quality (Fournier 2006; van der Werf 1996). This contributed to an unsustainable increase in yield, while pesticides and metabolites were spread throughout the environment with potentially negative impacts on ecosystems (Tilman et al. 2002) and on human health. Nowadays, despite progress in using ecological processes to manage agro-systems with less chemicals (Altieri 1995; Altieri and Nicholls 2000; Kogan 1998; Malézieux 2012; Rosset and Altieri 1997), in practice, the use of pesticides is still widespread and even in innovative practices such as no-till systems coupled with the use of herbicides (Alletto et al. 2010; Carof et al. 2007; Roger-Estrade et al. 2009).

Capel et al. (2001) analyzed the behavior of 39 pesticides at different scales in the USA and showed that the annual load of pesticides in streams as a percentage of use is usually less than 2 % in large catchments (>100,000 ha). However, even if the rates of pesticides reaching rivers are usually low in catchments, pesticides pollute environmental compartments and food, leading to sanitary (Hjorth et al. 2011) and eco-toxicological issues (Chapman and Stranger 1992; Desneux et al. 2007; Tanji 1993; Warren et al. 2003). The impact of pesticides on the environment ranges from ecosystem disruption to human health risks related to the contamination of drinking water and food (Cabidoche and Lesueur-Jannoyer 2012; Daam and den Brink 2009; Finizio et al. 2001; Kruhm-Pimpl 1993).

The main processes involved in the fate of pesticides are degradation, retention, volatilization, drift, atmospheric dispersion, runoff, and leaching (Calvet et al. 2005; van Dijk and Guicherit 1999; Holvoet et al. 2007; Schiavon et al. 1995; van der Werf 1996). Once applied, the transfer of pesticides in the catchment depends on catchment hydrologic characteristics (Abbott et al. 1986a; Blanchard and Lerch 2000). Modeling these processes is one way to account for the response of a catchment to the combination of agricultural practices, the effects of which are difficult to test experimentally at such a scale (Arnold et al. 1998).

A catchment outlet combines the effects of agricultural practices and natural processes occurring at the catchment scale, including the type, timing, and spatial position of the processes and practices (Fig. 1). Many field-scale models have

been developed to simulate pesticide transfer at field borders (Dubus and Surdyk 2006; Siimes and Kämäri 2003). In parallel, catchment scale models such as European Hydrological System (SHE) (Abbott et al. 1986b) or TOPMODEL (Beven and Kirkby 1979) have been developed. Catchment models provide a simplified virtual representation of catchment functioning. Most catchment models simulate water and pollutant transfers. With increasing concern about water pollution by agricultural pesticides, there is the crucial need for models that deal with both scales. It is a known fact that, due to emergent processes at the catchment scale, the functioning of a catchment is more complex than a simple linear combination of emissions at the field scale (Cerdan et al. 2004; Shaman et al. 2004; Sivapalan 2006). However, catchment scale models were not designed to take the effects of agricultural practices on catchment response into account. Hence, the issue of including the effects of field-scale agricultural practices in catchment scale models has led to the development of new models that can account for agricultural practices when estimating the contamination of streams by pesticides (Arnold et al. 1998).

As summarized by Kauark Leite (1990), pesticide transfer models at the catchment scale can serve several purposes: (a) estimating pollutant fluxes, (b) estimating the risk of exceeding a particular concentration, (c) describing and identifying transport mechanisms, (d) locating and quantifying the importance of pollution sources, and (e) evaluating the effects of agricultural practices on water quality. Assessing cropping system scenarios at the landscape scale is a major objective for agronomists (Martin et al. 2006; Meynard et al. 2001). Catchment scale models can help diagnose and identify combinations of practices and other environmental factors that contribute to water contamination by pesticides at the watershed outlet (Biarnes and Colin 2006; Luo and Zhang 2009). Catchment scale models may also be able to determine whether changes in practices will have a beneficial effect on water quality (Arabi et al. 2007). The results of the simulations can be used to categorize scenarios based on their potential effect on water quality (Tixier 2004; Tixier et al. 2007; Zhang and Zhang 2011). A major challenge today is designing management-oriented assessment tools that can be more easily used by catchment managers (Quilbé and Rousseau 2007), agricultural advisors (Bockstaller et al. 2008), or farmers themselves (Barreteau et al. 2008).

Although catchment scale models have been reviewed several times (Beckers and Degré 2011; Borah and Bera 2003; Holvoet et al. 2007; Payraudeau and Gregoire 2012; Quilbé et al. 2006), these reviews focused on processes rather than on agricultural practices. Knowledge about practices is needed in models so that agronomists, managers, and developers can simulate existing and innovative practices. Modeling knowledge about farming practices will also help identify further research needs to enable the representation of agricultural

Fig. 1 Examples of agricultural practices which affect pesticide transfers in catchments: pesticide application (a), dead mulch ground cover (b), plastic mulch ground cover (c). Catchments are combinations of spatial

units with different environmental characteristics resulting from practices (d) (photos from Lesueur-Jannoyer)

practices in catchment scale models. Here, we propose a conceptual framework to determine if and how pesticide transfer models represent the effects of agricultural practices on the contamination of water by pesticides.

2 Methodology

2.1 Model selection

The models we identified for review and associated references are summarized in Table 1. In the first step, we selected models representing whole catchments, not only specific catchment structures. Models were selected to represent the different types of catchment models identified in previous reviews: Following Quilbé et al. (2006), we selected management models (Soil and Water Assessment Tool (SWAT), annualized-Agricultural Non-Point Source (annAGNPS), Hydrological Simulation Program—Fortran (HSPF)), research models (MIKE SHE, Distributed Hydrological Modeling of Agrosystems (MHYDAS)), and multimedia models (SoilFug). Following Payraudeau and Gregoire (2012), MIKE SHE and MHYDAS represent physically based models; SWAT, annAGNPS, and

HSPF represent conceptual models; and an environmental indicator (I-phyBV) was added to our selection set. Because of the huge amount of data needed to run simulation models, researchers are particularly interested in developing methods that require fewer input data such as multimedia models (Mackay 2001) or environmental indicators. Environmental indicators have been optimized for management purposes which makes them good candidates for the assessment of practices by agronomists (Devillers et al. 2005; Maraite et al. 2004; Wohlfahrt et al. 2010). To ensure that the selected assessment tools were representative of their diversity, we searched the Web of Knowledge up to May 2012 using the following keywords: “[Topic=(model*) AND Topic=(pesticide*) AND Topic=(practice*) AND (Topic=(catchment*) OR Topic=(watershed*))]”. The results obtained confirmed our preselected list of assessment tools. For purposes of comparison, we completed the set of models with the geo-Pesticide Emission Assessment at Regional and Local scales (geoPEARL) model (a physically based research model) that assesses the contribution of practices to groundwater loading by pesticides at a regional scale. Finally, we searched for available documentation to validate the height assessment tools at the catchment scale: annAGNPS, geoPEARL, HSPF, I-phyBV, MHYDAS, MIKE

Table 1 Models and associated references

Models	References
annAGNPS	Young et al. 1994^a; Bingner et al. 2011^b; Young et al. 1989^c; Yuan et al. 2008^e
geoPEARL	Tiktak et al. 2003^{a,b}; Tiktak et al. 2004^a; Tiktak et al. 2002^{c,e}
<i>GLEAMS</i>	<i>Knisel and Walter 1993^{a,b}; Leonard et al. 1987^c; Knisel et al. 1995^d; Knisel et al. 1989^e; Magliola and Knisel 1992^e</i>
HSPF	Bicknell et al. 1996^{a,b}; Donigan et al. 1995^c; Mohamoud et al. 2010^d
<i>I-pest</i>	<i>van der Werf and Zimmer 1998^c; Roussel et al. 2000^e</i>
I-phyBV	Thiollet-Scholtus 2004^c; Wohlfahrt 2008^c
<i>MACRO</i>	<i>Stenemo and Jarvis 2010^d; Larsbo and Jarvis 2003^b; Jarvis et al. 1997^c</i>
MHYDAS	Charlier 2007^b; Moussa et al. 2002^c; Moussa et al. 2010^c; Moussa et al. 2003^e
MIKE SHE	DHI 2007a^a; DHI 2007b^b; Styczen et al. 2004^b; Abbott et al. 1986a, b^c; Refsgaard and Storm 1995^c; Styczen et al. 1999^e; de Bruyn et al. 2006^e
<i>PEARL</i>	<i>Tiktak et al. 2000^a; Leistra et al. 2001^b</i>
<i>PestLCI</i>	<i>Birkved and Hauschild 2006^c</i>
<i>PRZM</i>	<i>Suarez 2005^{a,b}; Carsel et al. 1985^c</i>
<i>R-pest</i>	<i>Tixier 2004^{b,e}; Tixier et al. 2007^{c,e}</i>
<i>RZWQM</i>	<i>Ahuja et al. 2000^b; Wauchope et al. 2004^b; Ma et al. 2001^{c,d}; Malone et al. 2004^e</i>
SoilFug	Barra et al. 1995^c; Barra et al. 2000^c; di Guardo et al. 1994^c
SWAT	Arnold et al. 2011^a; Neitsch et al. 2011^b; Arnold et al. 1998^c; Srinivasan et al. 1998^c; Arabi et al. 2008^d; Zhang and Zhang 2011^e

Catchment scale models are in bold; field-scale models are in italics

^a User manuals

^b Technical or theoretical guides

^c General or initial publications

^d Publication on practices

^e Model uses

SHE, SoilFug, and SWAT. To avoid unnecessary repetition, the term “model” is used hereafter to qualify all selected assessment tools including simulation models and indicators.

Analysis of the structure of the MIKE SHE, MHYDAS, and HSPF models showed that they were developed primarily at the catchment scale. The other models were based on previously developed pesticide transfer models at the field scale (Chemicals, Runoff, and Erosion from Agricultural Management Systems (CREAMS), Groundwater Loading Effects of Agricultural Management Systems (GLEAMS), PEARL, and I-pest). The field-scale models have been adapted so they can be incorporated in catchment scale models, and as a result, they do not exactly match the stand-alone field-scale versions. Two catchment scale models (HSPF and MIKE SHE) have been bridged to field-scale

models to improve their representation of field-scale practices and processes. Pesticide Root Zone Model (PRZM) was bridged to HSPF by the PZ2HSPF Bridge Program (Suarez 2005), and DAISY (Abrahamsen and Hansen 2000) and MACRO were bridged to MIKE SHE (van der Keur et al. 2011; Styczen et al. 1999). Pesticide transfer models at the field-scale and crop models coupled with pesticide transfer models at the catchment scale are summarized in Table 2.

In the second step, we selected field-scale models for review because they were developed specifically to assess the effects of agricultural practices on pesticides transfers at the field border and are used to generate inputs for catchment models. We found three field-scale models (Root Zone Water Quality Model (RZWQM), R-pest, and PestLCI) with documented descriptions of practice. As to our knowledge, they had not been associated with pesticide transfer models at the catchment scale; we also reviewed them for the purpose of comparison. GLEAMS is an update of CREAMS with improved groundwater capacities (Knisel and Walter 1980; Leonard et al. 1987), so we only reviewed GLEAMS.

For each model, we selected a set of documents including the manual, the technical guide, publications associated with the development of the model, and publications related to its use for diagnosis or simulation studies (Table 1). When the authors published a special paper to explain how to represent agricultural practices in the model, the paper was included in the set. Unfortunately, not all documents were available for the models we selected (Table 1). This finding revealed a lack of homogeneity in the framework associated with model development and documentation, especially for user manuals, and the focus of this review: publications on practices.

2.2 Conceptual framework

In agricultural catchments, pesticides may be applied on fields (Real 2004), on field borders such as hedges (Moonen and Marshall 2001), and on tracks and roads (Huang et al. 2004).

Table 2 Catchment scale models and associated field-scale models

Catchment models	Field-scale pesticide models	Field-scale crop models
annAGNPS	CREAMS	EPIC
geoPEARL	PEARL	WOFOST
HSPF	Included/PRZM	Generic
I-phyBV	I-pest	None
MHYDAS	Included	None
MIKE SHE	MIKE SHE AD/ MACRO/DAISY	Included/MACRO/ DAISY
SoilFug	Included	Simple
SWAT	GLEAMS	EPIC

Each line of the table shows the field-scale pesticide and crop models that have been integrated or bridged to each catchment model

As diffuse pollution results from pesticides applied on fields (Levillain et al. 2012), we focused on the effects of agricultural practices on the fate of pesticides applied on fields.

At field and catchment scales, the general mechanisms that influence pesticide transfers can be represented as shown in Fig. 2: (i) Agricultural practices modify variables describing environmental characteristics (such as soil hydraulic properties or ground cover) of one or more environmental compartments (such as soil or plants). (ii) Variables describing environmental characteristics modify the response of the simulated processes according to the variables defining the climate. (iii) The resulting hydrologic and biophysical processes modify environmental characteristics. For instance, tillage affects (i) soil hydraulic properties which, in turn, modify (ii) different hydrologic processes (leaching, runoff) that occur in soil after a rainfall event (Alletto et al. 2010). The resulting water fluxes modify (iii) the pesticide content and distribution in the soil due to leaching or runoff. In Fig. 2, decisional relationship arrows represent the farmer's decisions concerning which practices to use in a given field depending on its climatic and environmental characteristics. For instance, herbicide applications can use a threshold based on weed height, but no herbicide applications are performed on rainy days. In this review, we focused on the simulation of the effects of practices on points (i) and (ii) only. The effects of processes on environmental characteristics as well as decision models for applications of practices are not discussed in this article.

2.3 Selection of practices and processes

We review models at both the field and the catchment scales. The models have different objectives and thus do not simulate exactly the same categories of processes. Field models simulate production of flows but do not simulate flow transfers, whereas catchment models simulate both the production and transfer of flows. We took this difference into account in the selection of the practices and processes analyzed in our review. The relations between practices and processes analyzed in this review are not exhaustive but suffice to discuss the

conclusions which can be drawn by using our conceptual analysis framework. Holvoet et al. (2007) report that contamination of rivers can be significantly reduced by reducing pesticide use and by applying practices to control runoff and erosion, along with drift reducing measures. We thus chose to analyze the effects of practices on runoff/infiltration, erosion, and drift. These processes are produced at field scale and transferred at catchment scale making it possible to discuss the change in scale. The main environmental characteristics found to affect pesticide transfers toward the identified processes were ground cover, soil water content, the distribution of pesticides in the different environmental compartments, soil hydraulic properties, soil erodibility, and soil organic matter content (Alletto et al. 2010; Leonard 1990). The main field-scale practices found to affect the above-mentioned environmental characteristics were pesticide application, tillage, manure application, mulching, cover cropping, crop plantation, crop harvest, mowing, clearing, pruning, and irrigation (Alletto et al. 2010; Hartwig and Ammon 2002; Walter et al. 1979). We selected four types of practices based on their effects: (1) pesticide applications make pesticides available in the different environmental compartments; (2) tillage, which has drastic effects on most of the environmental characteristics that affect pesticide transfer (soil hydraulic properties, soil erodibility, soil ground cover, soil organic matter, and pesticide distribution in soil); (3) practices associated with the management of ground cover (tillage, impervious mulching, mulching using plant residues, cover cropping, crop plantation, crop harvest, mowing, clearing, and pruning), which make it possible to compare the models' representation of innovative practices (impervious mulching, plant residue mulching, cover cropping) with their representation of conventional practices (tillage); and (4) catchment practices that interact with pesticide flows. The catchment practices identified as affecting pesticide flow in catchments were buffer zones, waterways, ditches, tile drainage, and ponds (Reichenberger et al. 2007; Rice et al. 2007).

To conduct a broad yet in-depth analysis of the modeled agricultural practices, we selected specific relationships

Fig. 2 Relationships between agricultural practices and pesticide transfer related processes: (i) Agricultural practices modify variables describing environmental characteristics (such as hydraulic properties or ground cover). (ii) Variables describing environmental characteristics modify

the response of the simulated processes according to the variables defining climate. (iii) The resulting processes modify the environmental characteristics

between practices and processes (Table 3). Other processes or practices were not included in our in-depth analysis either because the lack of information on the effect of certain practices (retention, degradation) would spoil the comparison or because their representation was not a priority for catchment modelers (volatilization).

2.4 Data analysis

First, we compared models on the basis of whether they accounted for our subset of selected practices (pesticide application, tillage, and mulching) (Table 4). It is important to note that this study relies on a literature analysis only. None of the models we reviewed were tested. We analyzed the methods and scientific knowledge used to represent the effect of identified practices on runoff, infiltration, erosion, and drift according to our conceptual framework. Then, we classified our results under five points with illustrations of specific practices:

We found different levels of integration of practices in models. We discuss the levels of integration based on the effects of tillage on runoff through soil hydraulic properties and soil cover and the effects of tillage on erosion through erodibility (Section 3). We found different pesticide application practices represented in models as well as various tillage mixing algorithms and wondered about their effects on pesticide transfers (Section 4). We discuss whether models simulate innovative agricultural practices by analyzing practices related to ground cover management (impervious plastic mulching, mulching using plant residues, and associated cover cropping) (Section 5). We discuss problems of changes in scale by analyzing how space is represented in catchment

models and how drift and drift redeposition are modeled (Section 6). We also checked whether and how catchment practices (buffer zones and ditches) had been integrated in the models (Section 7).

In Section 4, we compare the algorithms used to represent the effects of tillage on pesticide distribution in the soil profile by simulating pesticide distribution in soil layers using the tillage algorithms found in the models. To this end, we simulated a moldboard plow tillage operation at 30 cm depth from an initial situation of 10 kg ha^{-1} of pesticides applied to the first 1 cm of the soil. For the simulation, the soil was represented as having 11 layers and a depth of 50 cm. The first layer was 10 mm deep, the second 40 mm, and the other eight were each 50 mm deep. Figure 4 presents the simulation results.

3 Levels of integration of practices

Table 4 summarizes the reviewed cropping system practices implemented in pesticide transfer models at both catchment and field scales. To illustrate the levels of integration of practices in the models, we focused on the effect of tillage on runoff and erosion through soil hydraulic properties, soil cover, and soil erodibility. Using the analytical framework depicted in Fig. 2, we found four levels of integration of the effect of a practice on processes related to pesticide transfers (Fig. 3):

Level 1: The process is not represented by the model. As a result, the effects of practices on the process cannot be represented. For instance, MACRO, PEARL, geoPEARL, I-pest, I-phyBV, PestLCI, RZWQM, and SoilFug models do not have an erosion module, which implies that tillage

Table 3 Relationships between practices, environmental characteristics, and processes analyzed in the review

Practices	Environmental characteristics	Processes	Sections
Tillage	Soil hydraulic properties	Runoff/infiltration	3.2
Tillage	Erodibility	Erosion	3.3
Tillage	Ground cover	Runoff/infiltration	3.2–5.1
Tillage	Ground cover	Erosion	3.3–5.1
Tillage	Pesticide vertical distribution in soil	Runoff/infiltration	4.1
Pesticide application	Amount of pesticides in environmental compartments	Various depending on models and compartments	4.2
Pesticide application	Amount of pesticide in air	Drift redeposition	6.2
Plastic mulching	Impervious ground cover	Multiple, no specific example	5.2
Crop residues mulching	Pervious ground cover	Multiple, no specific example	5.3
Cover crop mulching	Pervious ground cover	Multiple, no specific example	5.4
Ditch and waterway	Vegetative cover and size	Runoff and erosion interception	7.1
Buffer zone	Vegetative cover and size	Runoff and erosion interception	7.2

Each line corresponds to a relationship. The first column gives the practice, the second column gives the environmental characteristic affected by the practice, and the third column gives the process affected by the modification of the environmental characteristic. The last column indicates the sections of the article discussing each relationship

Table 4 Effects of cropping system practices on environmental characteristics affecting pesticide transfers in the reviewed models

Models	Pesticide application effects on		Tillage effects on		Mulching using					
	(1) Drift	(2) Dose partition	(3) Pesticide runoff and infiltration through pesticide distribution in soil	(4) Runoff and infiltration through ground cover	(5) Runoff and infiltration through soil hydraulic properties	(6) Erosion through erodibility	(7) Impervious mulch	(8) Ground cover by plant residues	(9) Crop growth and mixed cropping	(10) Pruning, clearing, and mowing
amAGNPS	–	SC	L3	L4	L4	L4	–	X	1	–
geoPEARL	–	SC	L4	L2	L3	L1	–	–	1	–
GLEAMS	X ^a	SC	L3	L4	L4	L4	–	X	I	–
HSPF	X ^a	SC P	L3–L4 ^c P	L3–L4 P	L3–L4 P	L3–L4 P	–	X P	1–1 P	–
I-pest	X ^b	SC	L2	L3	L3	L1	–	–	–	–
I-phyBV	X ^b	SC	L2	L3	L3	L2	–	X	NS	–
MACRO	X ^a	SC	L3	L2	L4	L1	–	–	I	–
MHYDAS	–	–	L3	L2	L3	L3	–	–	NS	–
MIKE SHE	X ^a M	S–SC DM	L3–L4 D–L3 M	L2–L2 D–L2 M	L3–L3 D–L4 M	L3–L1 D–L1 M	–	X D	1	–
PEARL	–	SC	L4	L2	L3	L1	–	–	I	–
PestLCI	X ^a	SC	L2	L2	L2	L1	–	–	I	–
PRZM	X ^a	SC	L4 ^c	L4	L4	L4	–	X	I	–
R-pest	–	S	L2	L4	L4	L4	–	X	B+W	X
RZWQM	X ^a	SCMulch	L4	L2	L4	L1	–	X	I	–
SoilFug	–	–	L2	L2	L2	L1	–	–	1	–
SWAT	X ^a	SC	L4	L4	L4	L4	–	X	Mult+W	X ^d

Catchment scale models are in bold; field-scale models are in italics. In column (9), number of simultaneous crops which can be simulated by the model

X taken into account in the model, – not taken into account in the model or undocumented, $L1$ level 1 of practice integration (process not simulated by the model), $L2$ level 2 of practice integration (process is independent from the environmental characteristic), $L3$ level 3 of practice integration (no simulation of the effect of the practice on the environmental characteristic but simulation of the effect of environmental characteristic on process), $L4$ level 4 of practice integration (practice effect on process is simulated by the model), NS not simulated but a value can be input manually by the user, P using PRZM as field model, D using DAISY as field model, M using MACRO as field model; S soil, C crop(s), $Mulch$ (compartments considered during the pesticide application partitioning algorithm); W weeds simulation, $Mult$ multiple crops (theoretically no limits), B specific to banana cropping systems

^a Loss only

^b Drift deposition estimation

^c Distribution possible only during pesticide applications

^d Partial representation

Fig. 3 The four levels of integration of the effect of agricultural practices on processes in models

operations do not affect pesticide transfers through erosion even though it is known that tillage affects soil structure hence favoring soil and soil-bound pesticide transfers (Alletto et al. 2010; Takken et al. 2001)

Level 2: The process is represented by the model, but the environmental characteristic has no effect on the process or, in continuous models, the environmental characteristic cannot be modified during the course of the simulation. For instance, SoilFug simulates the runoff process, but the process does not depend on soil hydraulic properties. PestLCI has a parameter that partially represents soil hydraulic properties, but it depends only on sand content of the soil and cannot be modified even though it is known that tillage affects soil hydraulic properties leading to modifications in runoff and infiltration processes (Cresswell et al. 1993; Wu et al. 1992).

Level 3: The process is represented and depends on an environmental characteristic. However, there is no module in the model to estimate the effect of the practice on the environmental characteristic concerned. For instance, HSPF, MHYDAS, MIKE SHE, and I-phyBV simulate runoff and infiltration. They have parameters that are presented as being modified by tillage practices. However, the value of the parameters has to be supplied by the user and is not simulated by a module in the model.

Level 4: Environmental characteristics and the process are fully integrated in the model. Environmental characteristic values are calculated from the application of practices and have direct or indirect effects on pesticide transfer processes. For instance, GLEAMS, MACRO, RZWQM, R-pest, PRZM, SWAT, and annAGNPS simulate the effect of tillage on soil hydraulic properties

which in turn affects the runoff and infiltration processes and the resulting pesticide transfers.

Table 4 shows that most models do not simulate erosion and are thus unable to assess the effects of any practice on pesticide transfers caused by erosion. Most field-scale models integrate the effects of tillage on runoff and infiltration at level 4. In catchment scale models, except for annAGNPS and SWAT, the integration of the effects of tillage is below level 4. Nevertheless, the levels of integration are improved by bridging catchment scale models to field-scale models (HSPF). We also found that the representation of time in a model constrains the level of integration of the effects of agricultural practices on processes (Section 3.1). Finally, we found that different models rely on the same method to simulate the effect of an agricultural practice on a process and that only a few methods integrate the practice at level 4 (Sections 3.2, 3.3, and 3.4).

3.1 Continuous and event models

Borah and Bera (2003), Quilbé et al. (2006), and Payraudeau and Gregoire (2012) divided catchment scale models into two categories: event models and continuous models. Event models simulate catchment response to a single rainfall event and are thus short-term response models, whereas continuous models simulate rainfall events as well as changes in the catchment between rainfall events. The resulting total simulation period can last from less than 10 years to more than 40 years (Borah and Bera 2004). Our conclusion is that event models (I-pest, I-phyBV, and MHYDAS) do not simulate the

Fig. 4 Comparison of the effects of the tillage algorithms found in models on the vertical distribution of pesticides in the soil profile. Tillage is a moldboard plow operation at 30 cm depth from an initial situation of 10 kg/ha of pesticides applied to the first 1-cm layer of the soil. The soil was represented as having 11 layers and a depth of 50 cm. The first layer was 10 mm deep, the second 40 mm, and the other eight were each

50 mm deep. **a** Initial situation or models without tillage algorithm. **b** Pesticide Emission Assessment at Regional and Local scales (*PEARL*) tillage algorithm. **c** Soil and Water Assessment Tool (*SWAT*) and Root Zone Water Quality Model (*RZWQM*) algorithm, the mixing efficiency parameter is set to 0.95 as indicated in the documentation of the models. **d** DAISY (not an acronym) algorithm

effects of agricultural practices on environmental characteristics. In such models, the initial values of environmental characteristics have to be estimated or measured prior to the simulation (integration at level 3). For instance, MHYDAS associates soil-saturated hydraulic conductivity values with different cropping system components, such as tilled fields or untilled fields, prior to the calculation (Moussa et al. 2002); I-phyBV indicator values are inferred from MHYDAS simulation results using the Monte Carlo procedure (Wohlfahrt 2008) or expert parameterization based on soil hydraulic conductivity at saturation characteristics (Thiollot-Scholtus 2004). Conversely, the 14 continuous models (annAGNPS, geoPEARL, GLEAMS, HSPF, MACRO, MIKE SHE, PEARL, PestLCI, PRZM, R-pest, RZWQM, SoilFug, and SWAT) make it possible to integrate practices at level 4 as they at least simulate changes in one environmental

characteristic (crop cover). However, this is not the case for all processes, as only six models integrate the effect of tillage on runoff by incorporating crop residues at level 4 (annAGNPS, GLEAMS, PRZM, RZWQM, R-pest, and SWAT) and only five integrate the effect of tillage on erosion by modifying the erodibility characteristic at level 4 (annAGNPS, GLEAMS, PRZM, R-pest, and SWAT) (Table 4).

3.2 Tillage and runoff

Three methods are used to produce runoff in models. The first is the curve number method (USDA 1986). The curve number is a lumped parameter that includes the effect of land use and surface conditions, among other characteristics (Ponce and Hawkins 1996). Surface conditions include the effects of

ground cover. GLEAMS, SWAT, annAGNPS, and PRZM use a curve number parameter to simulate runoff. The curve numbers are estimated using the values available in USDA (1986), which were recently updated (USDA 2012) and include the effects of both soil hydraulic properties and ground cover (level 4).

The second is the EPIC method. RZWQM and MACRO solve Richards' equation to produce runoff. More information on methods used to simulate water and pollutant flows in soil macropores is available in Simunek et al. (2003) and in Köhne et al. (2009a, b). RZWQM and MACRO require soil hydraulic properties and use the same algorithm to estimate changes in soil hydraulic properties after tillage. Soil hydraulic properties rely on the soil bulk density, which is the result of tillage operations and soil reconsolidation. In both models, the method used to predict soil bulk density after tillage is based on the EPIC model (Williams et al. 1984) which uses a tillage intensity factor and a consolidation bulk density. The EPIC method comes with tillage intensity factors for various tillage tools (Rojas and Ahuja 2000; Williams et al. 1990). The EPIC method is thus level 4 for soil hydraulic properties, but for runoff through ground cover is only level 2, since ground cover is not represented as affecting runoff. In HSPF, ground cover restricts the velocity of runoff and reduces the total quantity of runoff by allowing more time for infiltration. HSPF has no tillage module (level 3) unless coupled to PRZM (level 4).

The last method comes with R-pest. Runoff is calculated as a function of soil hydraulic properties (soil compaction), tillage direction, and ground cover. All tillage practices have the same effect on the soil compaction indicator and ground cover by decreasing their values to the minimum values (0 and 0 %). Tillage is thus integrated at level 4 but relies on extreme modifications of environmental characteristics.

3.3 Tillage and erosion

Models that use the Universal Soil Loss Equation (Wischmeier and Smith 1978) or its derivative, the Revised Universal Soil Loss Equation (Renard et al. 1997) to simulate erosion integrate tillage effects at level 4. In these methods, two factors of the equation, C and P , stand for the effect of the cropping system and the erosion control practices on soil erodibility, respectively. The C factor is modified by tillage practices, whereas the P factor stands for more structural tillage practices (contour tillage, strip cropping). AnnAGNPS, GLEAMS, and PRZM use a surface roughness coefficient, which is modified by tillage, to calculate the C coefficient. Databases that can be used for this calculation are available in Sharpley and Williams (1990), Wischmeier and Smith (1978), or the specific model documentation. The Universal Soil Loss Equation is used by models that use curve numbers to simulate runoff. As for runoff, R-pest

integrates the effect of tillage on erosion at level 4 using extreme modifications of soil compaction and soil cover.

MIKE SHE and MHYDAS use physically based methods to represent soil erosion. MHYDAS uses MHYDAS-EROSION (Gumiere et al. 2010). The MIKE SHE erosion module is based on the European Soil Erosion Model (Morgan et al. 1998). In both models, erosion is presented as being modified by tillage, but there is no module to estimate the effects of tillage on erosion (level 3). Instead, models use calibrated data or measured data on fields that are tilled or not tilled (Gumiere et al. 2010). In MHYDAS, the soil cover is not represented, but its effect on erosion can be taken into account using the Manning roughness coefficient. MIKE SHE reduces rainfall energy by crop canopy interception.

3.4 Data requirements

Despite the large number of studies reviewed by Alletto et al. (2010) that report the effects of tillage on the fate of pesticides, tillage integration at level 4 is limited to global trends of cropping systems such as conventional tillage and conservation tillage. This confirms the lack of available knowledge to parameterize the effects of tillage on pesticide transfers. For instance, the curve number and the Universal Soil Loss Equation can be used to estimate the effect of conventional and conservation tillage on runoff and erosion, respectively. Each tillage modality works with two possible tillage directions: straight rows or contouring. Other authors integrate tillage at level 4 using only one tillage modality leading to modifications of environmental characteristic to extreme values (R-pest). Other methods with the highest tillage resolution (choice of tool) such as the EPIC method were perhaps not integrated in the catchment scale models because these models focus on the effect of tillage on runoff using only soil hydraulic properties and do not consider the other effects of tillage on runoff (ground cover) or on other processes (erosion).

4 Pesticide distribution

When pesticides are applied to fields, the dose is split between the different environmental compartments (plant, soil, air, mulch). The distribution of pesticides in the field influences whether they are subject to transfer and degradation processes such as washoff, runoff, volatilization, leaching, photodegradation, bacterial metabolism, and hydrolysis (Barriuso 2004). For instance, pesticides that are incorporated into the soil are less exposed to volatilization and runoff than pesticides applied on the surface of the soil (Larson et al. 1995). Pesticides applied on plants are subject to washoff, photodegradation, and plant absorption, whereas pesticides in the soil are not (Calvet et al. 2005; Galiulin et al. 2002; Norris 1974). Pesticide

distribution at field scale determines the pathways of the pesticide to the catchment outlet. For instance, Charlier et al. (2009) showed that, in the specific case of a catchment with shallow groundwater connected to surface water, pesticide transfers by runoff cause peaks of high pesticide concentrations in the stream, whereas shallow groundwater flows buffer pesticide concentrations by diluting and spreading pesticides over time leading to chronic contamination of the stream. To illustrate the potential effects of model structures and model algorithms on cropping systems assessment, we present practices that directly affect the distribution of pesticides in fields: tillage (Section 4.1) and pesticide applications (Section 4.2).

4.1 Tillage effects

To simulate the redistribution of chemicals during tillage, models have to use a layered representation of the soil. Seven models do not represent the effect of tillage on pesticide redistribution in the soil (annAGNPS, GLEAMS, I-pest, I-phyBV, PestLCI, R-pest, and SoilFug). Among them, four models (I-pest, I-phyBV, R-pest, and SoilFug) have no layered representation of the soil. These models cannot represent the vertical heterogeneity of soil pesticide contents. AnnAGNPS, GLEAMS, and PestLCI have a layered soil representation but either lack a module for representing soil mixing by tillage (PestLCI) or they have one for nutrients but not for pesticides (annAGNPS and GLEAMS).

PEARL, SWAT, RZWQM, MACRO, and PRZM have a pesticide mixing module. The simplest module for tillage mixing is the one in PEARL. The module mixes the amount of pesticides uniformly throughout the tillage depth (Fig. 4b). Only tillage depth is needed in this case. The SWAT and RZWQM mixing modules (Fig. 4c) require two parameters to estimate chemical mixing in soil layers: depth and mixing efficiency. The efficiency is the fraction of pesticide mixed uniformly in the tilled layers. When coupled to the DAISY field model, the MIKE SHE model has a mixing module with two basic actions: mix and swap. With the mix effect, pesticides are averaged throughout the tillage depth. Swap simulates the inversion effect of tillage. When swap is enabled, DAISY considers two equal sub-layers that are swapped around by tillage after being mixed separately (Fig. 4d). PRZM and MACRO consider the effect of tillage on pesticide distribution in the soil only if tillage is performed on the same day as pesticide application. In these models, subsequent tillage operations have no effect on pesticide distribution in soil layers. Suarez (2005) gives the links between tillage practices and the different tillage algorithms used by these two models.

Tillage algorithms result in different vertical distributions of pesticides, making different amounts of pesticide available for the transfer processes such as runoff and percolation in the soil. Here we consider that only pesticides in the top layer are

available for runoff. After the operation presented in Fig. 4, the soil surface holds 0.33 kg ha^{-1} of pesticide with PEARL. The RZWQM and SWAT algorithm resulted in more than twice this amount (0.81 kg ha^{-1}) at the soil surface whereas the DAISY algorithm does not make any pesticides available to the soil surface (0 kg ha^{-1}). Models with no tillage algorithm for pesticides assume the total amount of pesticides applied (10 kg ha^{-1}) is available for runoff. These differences can lead to simulations of contrasting behaviors of pesticides in the catchment by modifying the transfer pathways.

4.2 Pesticide application practices

Pesticide application practices lead to several different distributions of the pesticides applied to the different compartments such as crops, cover crops, weeds, and residues as well as their distribution in the soil profile. In the models we reviewed, we identified different height representations of pesticide application practices affecting pesticide distribution in environmental compartments (Table 5).

Above canopy broadcast application is a practice included in all continuous models as well as in indicators. It stands for spraying pesticide uniformly above the crop canopy. In models, the amount of pesticide applied is linearly intercepted by the crop on the basis of crop coverage with the remaining fraction reaching compartments located under the crop, i.e., the mulch and the soil. In GLEAMS, the intercepted fraction has to be indicated manually. PRZM and MACRO account for a linear or an exponential filtration by crop canopy. Among the models reviewed, only RZWQM simulates the interception of pesticides by a mulch of crop residues before they reach the soil (Table 5).

Soil broadcast means the pesticide is directly applied on the soil. In models, this is represented by directly adding non-drifted pesticides to the soil. In this case, no interception by any environmental compartments other than soil is simulated. If soil is layered, pesticide is added to the first centimeter of soil (GLEAMS, annAGNPS, and RZWQM); pesticide is distributed to 4 cm, linearly decreasing with depth (PRZM and MACRO); or pesticide is added to the top computation layer (PEARL and geoPEARL). If soil is not layered, pesticide is homogeneously mixed in the soil.

Foliar application means the pesticide is applied to the leaves using manual or vertical mechanical pulverization. In models, it is simulated by adding non-drifted pesticides to the crop compartment only.

The use of *slow release* (microencapsulated) pesticide formulations (Shasha et al. 1976; Sinclair 1973) is simulated only in RZWQM using a time-dependant amount of pesticide available from an initial stock.

Injection in the soil is the application of the pesticide at a certain depth in the soil with or without pressure (All and Dutcher 1977). It is usually used for fumigation purposes. In

Table 5 Pesticide application practices available in models

Models	Above canopy broadcast	Soil broadcast	Incorporation with tillage	Foliar application	Application in irrigation water	Slow release application	Injection in soil	Band or localized application
annAGNPS	X	X	X	X	–	–	–	–
geoPEARL	X	X	X	X	–	–	X	–
<i>GLEAMS</i>	<i>X</i>	<i>X</i>	<i>X</i>	<i>X</i>	<i>X</i>	–	<i>X</i>	<i>X</i>
HSPF	See PRZM via PZ2HSPF							
<i>I-pest</i>	<i>X</i>	–	<i>X</i>	–	–	–	–	–
I-phyBV	X	X	X	–	–	–	X	–
<i>MACRO</i>	<i>X</i>	<i>X</i>	<i>X</i>	–	–	–	<i>X</i>	<i>X</i>
MHYDAS	Not documented							
MIKE SHE	X^b	–	–	–	–	–	–	–
<i>PEARL</i>	<i>X</i>	<i>X</i>	<i>X</i>	<i>X</i>	–	–	<i>X</i>	–
<i>PestLCI</i>	<i>X</i>	–	–	–	–	–	–	–
<i>PRZM</i>	<i>X</i>	<i>X</i>	<i>X</i>	–	–	–	<i>X</i>	<i>X</i>
<i>R-pest</i>	–	<i>X</i>	–	–	–	–	–	–
<i>RZWQM</i>	<i>X^a</i>	<i>X</i>	<i>X</i>	<i>X</i>	<i>X</i>	<i>X</i>	<i>X</i>	–
SoilFug	Not documented							
SWAT	X	–	X^c	–	–	–	–	–

Catchment scale models are in bold; field-scale models are in italics

X taken into account in the model, – not taken into account in the model or undocumented, *Above canopy broadcast* the pesticide is sprayed uniformly above the crop canopy, *Soil broadcast* the pesticide is directly applied on the soil, *Foliar application* the pesticide is applied to the leaves using manual or vertical mechanical pulverization, *Application in irrigation water* the pesticide is diluted in irrigation water, *Slow release application* the formulation of the pesticide results in a slow release of the pesticide in or on soil, *Injection in soil* the pesticide is applied at a certain depth in the soil, *Band or localized application* the pesticide is applied in parallel bands or in specific places such as on or between the rows

^a Pesticide interception by crop residues

^b Using DAISY as field model

^c Only after an above canopy broadcast application

models, it is simulated by concentrating pesticides at a specific depth in the soil.

Band application and localized application means the pesticide is applied in parallel bands or in specific places such as on or between the rows. In GLEAMS, band application decreases the total amount of pesticide applied to fields compared to a broadcast application (Knisel et al. 1995). It accounts for the ratio of the treated area and the total area of the field. In MACRO and PRZM, however, localized pesticide applications attracted our attention. Indeed, the horizontal distribution of pesticides on fields resulting from localized applications is represented by a vertical depth-dependant distribution of pesticide in the soil profile (Suarez 2005). These two models use their conceptual vertical discretization to represent the effect of practices leading to heterogeneous horizontal distribution of pesticides in the soil.

Even if an application method is taken into account, its effect on pesticide transfers relies on the conceptual compartmentalization of the model. For instance, RZWQM is the only model we reviewed in which mulch intercepts pesticides. The other models do not simulate mulch or do not simulate

pesticide interception by mulch (Tables 4 and 5). This impacts the whole simulation of pesticide fate as the pesticides in these different environmental compartments are not subject to the same processes.

5 Innovative practices: ground cover management

Ground cover is a key environmental characteristic affecting pesticide transfer processes such as runoff, volatilization, and erosion (Alletto et al. 2010; Antonious and Byers 1997; Bartley et al. 2006; Foltz 2012; Gish et al. 1995). Ground cover can take the form of pervious or impervious mulches, and these have contrasting effects on pesticide transfers. Pervious mulch made of dead or living plants reduces runoff (Dabney 1998; Findeling et al. 2003) whereas impervious mulches (such as plastic mulch) favor runoff (Rice et al. 2001). Pervious mulch results from a combination of practices and processes such as planting a crop and a cover crop, the growth and development of both along with spontaneous weeds. Weeding or mowing transforms living mulch into dead

mulch if not removed. Tillage incorporates mulches into the soil with varying degrees of efficiency. To assess whether the models simulate innovative cropping systems and compare them to conventional ones, we analyzed the effects of practices affecting ground cover in both catchment and field-scale models (Table 4): tillage (Section 5.1), plastic mulching (Section 5.2), “dead” mulching (Section 5.3), and cover cropping and intercropping (Section 5.4).

5.1 Tillage and ground cover

Ground cover is directly affected by tillage, by the burying of plants and plant residues. In SWAT, MIKE SHE–DAISY, and RZWQM, the effect of tillage on ground cover is simulated in the same way as chemical redistribution in the soil. The mixing module is used to estimate soil cover as a result of biomass redistribution in the soil. GLEAMS, annAGNPS, and PRZM use a residue incorporation efficiency parameter to determine the percentage of residue and plant material incorporated into the soil and left on the surface after a tillage operation (Knisel and Walter 1980; Knisel and Walter 1993). R-pest has only one tillage operation in its database, and it decreases soil cover by weeds and residues to 0 % (Tixier 2004). MACRO, PEARL, PestLCI, and SoilFug do not simulate residues on the soil surface. MIKE SHE or HSPF can take the effect of tillage on ground cover into account by bridging pesticide transfer models at the field scale to these two catchment scale models. The effect of tillage on ground cover is simulated by half the models reviewed (Table 4), depending on the modelers’ objectives.

5.2 Plastic mulch

The most widely used impervious mulch is plastic, and its use has increased dramatically in the last 10 years (Kasirajan and Ngouajio 2012). It is mainly used for weed control in vegetable crops (Rice et al. 2001) and pineapple (Dusek et al. 2010). Impervious mulch favors runoff from covered fields. Due to its high cost, it is used for small area with high-income crops. However, none of the models we reviewed had available parameters or modules to simulate the effects of impervious mulch on the water budget or on the fate of pesticides. However, Dietrich and Gallagher (2002) showed extremely high concentrations of pesticides ($>100 \mu\text{g L}^{-1}$) in runoff water from tomato fields covered with plastic mulch which might be explained by the fraction of pesticide washed off leaves but not intercepted by the soil during runoff. In the case of pesticides that only very weakly bind to plastic, runoff can be enriched by the fraction of pesticides that are deposited on the mulch during application. For this reason, plastic mulching has been described as favoring pesticide transfers. Nevertheless, such effects are not included in pesticide transfer models either at the catchment or field scale.

5.3 Dead mulch

Mowing, clearing, pruning, harvesting, and weeding remove plant biomass from a living plant whether it be a crop, a cover crop, or a weed. The biomass can either be removed from the field or feed the pool of residues that remains on the soil surface. In the first case, the overall soil cover is depreciated, whereas in the second case, living mulch is converted into dead mulch and the plant residues undergo degradation (Raphael et al. 2012; Ripoché et al. 2008). GLEAMS, RZWQM, R-pest, PRZM, SWAT, annAGNPS, DAISY, and HSPF can simulate crop residues (Table 4), but not all models simulate the impact of a crop residue cover on pesticide transfers. For instance, in DAISY for MIKE SHE, crop residues are simulated to estimate changes in the organic matter pool but were not found to have an effect on hydrologic or pesticide transfer processes through ground cover. R-pest and SWAT are the only two models that simulate the generation of dead mulch by practices other than harvesting. SWAT, however, has only a partial support for the different practices. They can be simulated by combinations of simpler unitary operations with overridden parameters. Mulching crop residues during the crop cycle is not directly considered in the models (except with R-pest), thus confirming a lack in the representation of agricultural practices associated with ground cover in pesticide transfer models at both the field and catchment scales.

5.4 Crops, weeds, and cover crops

Ground cover is affected by crops, weeds, and cover crops. Except I-pest, I-phyBV, and MHYDAS, all the models reviewed simulate the growth of at least one crop associated with agricultural practices.

Mixing crops has potentially beneficial effects on environmental impacts and increases productivity (Malézieux et al. 2009). To integrate these effects of mixing crops, a model is needed that simulates the growth of several crops at the same time as well as their interactions. However, mixtures of crops and crop–weed associations are not widely represented in most crop models (Malézieux et al. 2009). Among catchment scale models, only SWAT can simulate mixing crops (Table 4). R-pest coupled with SIMBA enables a simple dynamic simulation of ground cover by weed growth under a banana canopy. A more complex support to simulate the growth of a cover crop has recently been developed for SIMBA (Tixier et al. 2011). I-pest and I-phyBV make it possible to indicate percentage soil cover by weeds, cover crops, and associated crops but do not simulate their growth. A major limitation of the pesticide transfer models at the field and catchment scales is that their crop models do not simulate mixed cropping, cover cropping, or weed management.

6 Upscaling practices

6.1 Space representation

Three classifications are usually given for spatial representation in catchment scale models: (a) lumped models, (b) distributed models, and (c) semi-distributed models (Beckers and Degré 2011; Gárfias et al. 1996). Lumped models are unable to account for the position of cropping systems within the watershed. However, they can be used on small catchments to represent pollutant transfers in groundwater using residence time distribution in the aquifers (Farlin et al. 2013). Distributed models split the catchment into units of fixed size usually by using a square grid (MIKE SHE, AGNPS) or a triangular grid (Julien et al. 1995). Spatial representation in distributed models is a complex affair concerning landscape elements that are smaller than the grid resolution. This is usually the case of linear entities, such as roads and ditches, as well as small areal entities such as buffer zones which have been shown to affect flows in watersheds (van Dijk et al. 1996; Jones et al. 2000). Semi-distributed models represent a watershed as a combination of lumped units usually called hydrologic response units or homogenous land units. These units are to be considered homogeneous with respect to their environmental characteristics (usually slope, soil type, and cropping system). In fact, and especially when modeling large watersheds, homogeneous units usually include a variety of cropping systems, leading to drastic simplifications in cropping system diversity within the homogeneous units. The difference between distributed and semi-distributed models is fuzzy as a distributed model grid considers lumped parameters. The distributed characteristic of a model depends on the ratio of the grid size to the size of the watershed (Bathurst 1986). This determines whether the model can separate agricultural fields or combines cropping system diversity under a unique value.

Over and above the size of the units and the regularity of the grids of distributed and semi-distributed models, the most astonishing difference in spatial representations in catchment scale models is related to the interactions between spatial units (“the interacting unit models”). Four of the models (HSPF, MIKE SHE, MHYDAS, I-phyBV) we reviewed simulate spatial interactions: Pesticides and water flows produced by a spatial unit enter the next spatial unit in the flow path and are subject to the processes that occur in the neighboring spatial unit. The discretization method proposed by Lagacherie et al. (2010) in Geo-MHYDAS uses an irregular grid but enables interactions between spatial units such as inflow interception by defining a topological organization of units within catchments. Such advances make it possible to generate space discretization to account for different types of spatial units (channels and fields for instance) while allowing spatial interaction between units on pesticide flows.

6.2 Drift modeling

The direct loss of pesticides during their application is called drift. This loss can pollute the vicinity of the field including streams, grass strips, or other fields. Application methods and the height of pulverization are the main factors that determine the amount of pesticides that drift during application taken into account by models (Birkved and Hauschild 2006; Wauchope et al. 2004; van der Werf and Zimmer 1998). Models can be classified in three groups depending on the way they handle drift (Table 4). Drifted pesticides may be represented as leaving the system (SWAT, GLEAMS, RZWQM, PestLCI, PRZM, and HSPF with the PZ2HSPF bridge), as being re-deposited as a function of distance from the field (I-pest and I-phyBV), or may simply not be taken into account (R-pest, annAGNPS, MIKE SHE, SoilFug). We found no information in MHYDAS or PEARL even though the drift process is mentioned in PEARL documentation (Leistra et al. 2001). Models that consider drift to leave the system use a pesticide application efficiency factor. In these models, the efficiency of pesticide application is the fraction of pesticides reaching the field, with the drifted part being lost. Values proposed for estimating drifted fractions in models that do not consider redeposition are substantial. Wauchope et al. (2004) estimate drift to range from 40 to 55 % of the amount of pesticides applied. Such values are confirmed by values ranging from 20 to 50 % of the applied dose (Maybank et al. 1978; Ravier et al. 2005).

At the catchment scale, the objective of calculating drift is estimating pesticide deposition on surrounding fields and rivers. Models considering drift deposition use the Ganzelmeier estimation method (Ganzelmeier et al. 1995) but only account for redeposition in rivers. Estimation of pesticide deposition is given as a function of distance from the field, the application technique, and the height of application. I-pest and I-phyBV use this method to estimate pesticide drift reaching the river (Thiollet-Scholtus 2004; van der Werf and Zimmer 1998). More recently, SWAT was adapted by Holvoet et al. (2008) to deal with direct losses and redeposition during pesticide applications also using the Ganzelmeier method. However, this has not yet been incorporated in the current version. The other catchment models fail to use the drift outputs from the field-scale models as inputs, e.g., pesticide redeposition, when modeling catchment processes. This shows that the change in scale needs to be better addressed in catchment models. Drift redeposition in catchments models will have to account for the organization and characteristics of the landscape when assessing the effects of drift on streams. Trees or other tall crops acting as buffers are not taken into consideration by the Ganzelmeier method in drift interception even though they can intercept a significant part of pesticide drift (Hewitt 2001; de Schampheleire et al. 2008). In their literature review, Ucar and Hall (2001) reported a lack of standard methodology to assess the effect of physical barriers on pesticide drift. Drift models have been developed to estimate the contamination of unwanted

targets by pesticides (Ellis and Miller 2010; Gil and Sinfort 2005). One of the next moves in catchment scale modeling should be to simplify and integrate landscape scale drift models.

Drift is the most weighted parameter determining river contamination risk in I-pest even for orchard systems. This is not in accordance with the lower influence of drift than of runoff in river contamination found in orchard systems (Schulz 2001) or with authors who report little influence of drift on stream water quality in open cereal cropping areas (Kreuger 1998). The I-pest indicator is considered at its unfavorable value when the drifted fraction reaching the river is higher than an arbitrarily selected value of 1 % (van der Werf and Zimmer 1998). To better account for the effect of drift on surface water contamination, the stream discharge—or at least the length and the width of the stream—should be taken into consideration.

7 Practices at the catchment scale

Catchment practices are structures that are integrated in the landscape. They modify the behavior of pesticides before they

reach the catchment outlet. In model documentation, we found information on buffer zones, drainage ditches and waterways, water bodies (ponds), tile drainage, and irrigation practices (Table 6). In the following sections, we show that the management of catchment structures needs to be better taken into account in models. We also found that not all models simulate the remobilization of pesticides intercepted by catchment structures. To illustrate these results, we compare the effects of drainage ditches, grassed waterways (Section 7.1) and buffer zone areas (Section 7.2) on pesticide transfers in the different models.

7.1 Ditches and waterways

The objectives of creating drainage ditches and grassed waterways are to intercept runoff and to favor water and pesticide infiltration while routing flow to the outlet. The vegetative cover of ditches and waterways is a key factor in pesticide interception because plants retain pesticides (Moore et al. 2001, 2011). On the contrary, non-vegetated ditches and gullies favor quick pesticide routing to the permanent hydrographic network, leading to pesticide contamination peaks.

Table 6 Catchment practices interacting with pesticide transfers available in models

Models	Catchment practices				Irrigation		
	Buffer zone	Drainage ditches	Waterbodies	Tile drainage	Irrigation	Chemicals in irrigation water	Water removal from source
annAGNPS	X^b	X	X	X	X	X	–
geoPEARL	–	X	–	X	X	X	–
<i>GLEAMS</i>	–	–	–	–	<i>X</i>	–	–
HSPF	X	X	X	–	X^e	–	–
<i>I-pest</i>	–	–	–	–	–	–	–
I-phyBV	X	X	–	X	–	–	–
<i>MACRO</i>	–	–	–	<i>X</i>	<i>X</i>	–	–
MHYDAS	X	X^c	–	X^c	–	–	–
MIKE SHE	X	X	X^d	X	X	–	X
<i>PEARL</i>	–	<i>X</i>	–	<i>X</i>	<i>X</i>	<i>X</i>	–
<i>PestLCI</i>	–	–	–	–	<i>X</i>	–	–
<i>PRZM</i>	<i>X^a</i>	<i>X</i>	–	–	<i>X</i>	–	–
<i>R-pest</i>	–	–	–	–	<i>X</i>	–	–
<i>RZWQM</i>	–	–	–	<i>X</i>	<i>X</i>	–	–
SoilFug	–	–	–	–	X	–	–
SWAT	X	X	X	X	X	X	X

Catchment scale models are in bold; field-scale models are in italics

X taken into account in the model, – not taken into account in the model or undocumented

^a Using PRZM-BUFF

^b Coupling with the Riparian Ecosystem Management Model

^c Using MHYDAS-DRAIN

^d Using MIKE 11

^e Using PRZM as field model

Three models use drainage ditches to simulate the routing of excess water to the hydrographic network only (geoPEARL, MIKE SHE, and MHYDAS). MHYDAS uses MHYDAS-DRAIN to represent ditches (Tiemeyer et al. 2007). The module has been used to test the effect of ditch networks on hydrology (flow routing and reinfiltration) but not on pesticide behavior (Levavasseur et al. 2012). None of the three models simulate the effect of a grassed ditch on pesticide removal from water and sediment flow. In these models, groundwater drainage is usually associated with tile drainage. As a result, in all three models, ditches favor fast pesticide flows to the river network. Models should be selected knowing that not all models that simulate ditches were designed to simulate pesticide interception by ditches.

Ditches and waterways in SWAT, annAGNPS, HSPF, and I-phyBV remove pesticides. In annAGNPS and HSPF, the effect of grassed waterways is parameterized using the channel module (LimnoTech 2010; Mohamoud et al. 2010). All four models make it possible to specify the length of ditches to assess their effect on pesticide removal. The width (HSPF, SWAT), the shape (HSPF), and the cover (HSPF, I-phyBV, and SWAT) of the waterways are used to determine pesticide interception effectiveness. Nevertheless, we found no modules that accounted for the management of ditches or waterways in the models or for the natural evolution of their ground cover.

7.2 Buffer zones

Buffer zone is a generic term to define non-channelized areas that intercept runoff, sediments, and pesticides due to a high vegetative or dead mulch coverage (Barling and Moore 1994). These zones are assumed to produce very little runoff and erosion. Three main types of buffer zones exist: buffer grassed strips, hedges, and riparian zones. Even though any correctly managed land can act as a buffer zone, these three zones intercept runoff, pesticides, and sediments (Campbell et al. 2004; Carluer et al. 2008; Lacas et al. 2005, 2012; Lin et al. 2002; Madrigal et al. 2002; Madrigal 2004; Passeport et al. 2013; Tortrat 2005). Except geoPEARL and SoilFug, all the catchment scale models we reviewed have been used to simulate the effect of buffer zones on pesticides, runoff, or erosion. While the AGNPS model (event model used as a basis of annAGNPS) simulates the buffer zone effects of sediments and attached pesticides (Vennix and Northcott 2004), annAGNPS does not. Bridging annAGNPS with the Riparian Ecosystem Management Model (REMM) is a way to simulate the effect of buffer zones (Yuan et al. 2007). AnnAGNPS-REMM simulates only riparian zones, which limits the spatial distribution of buffer zones in the catchment. Among pesticide transfer models at the field scale, only PRZM simulates buffer zones using the PRZM-BUFF model (Winchell and Estes 2009).

HSPF, MIKE SHE, I-phyBV, and MHYDAS are interacting unit models. Buffer zones are simulated by the generic field module of the model. In this case, any piece of land is potentially a pesticide interceptor and emitter at the same time. The size of buffer zones is constrained by the minimum size of the unit area accepted by the model. Water and pollutant interception depends on environmental characteristics which can be modified by the practices available in the model. In SWAT, no interaction between hydrologic response units can be simulated. Buffer zones are part of the hydrologic response units; they interact with the runoff generated by the unit, but not with runoff generated by upland units. In SWAT, a buffer zone can only intercept flows generated by one hydrologic response unit while models that simulate inflows in each spatial unit account for larger contributing areas corresponding to the watershed whose outlet is the buffer zone.

In continuous models, two contrasting representations of pesticide interception by buffer zones exist. HSPF and MIKE SHE represent conservative pesticide interception, which means that the next rainfall event remobilizes previously intercepted pesticides. In contrast, SWAT pesticide interception by buffer zones is not conservative. The removed fraction leaves the system. This is not in agreement with Lacas et al. (2005) and Barling and Moore (1994), who report that pesticides intercepted by buffer zones move to the subsurface or are desorbed from the soil surface. Thus, when simulating the effects of buffer zones, users must carefully check that the model's assumption will not lead to an underestimation of pesticide pollution at the catchment outlet.

8 Conclusions

This review helped identify the improvements required to better account for the effects of agricultural practices on pesticide transfers. We also provide some recommendations to help model users select an appropriate model depending on their objectives:

1. The change in scale is poorly addressed, as representations of pesticide applications on drift kept the original field-scale representation in all models except I-phyBV. Drift redeposition has been addressed in SWAT but is not yet included in the current version of the model. Drift needs to be better integrated in catchment models.
2. The integration of innovative practices is a necessary step forward in field and catchment models to ensure models are capable of assessing innovative cropping systems. Plastic mulches and associated cover cropping practices are already integrated in crop models such as STICS (Brisson et al. 2009), the cropping system representations of which may serve their improvements in pesticide transfer models at the field and catchment scales.

3. Using the conceptual framework proposed in this article, model users and developers will be aware of both the effects of practices represented by models and of those which are not. Its use will make descriptions of the effects of practices clearer, which, in turn, will make the selection and development of models easier.
4. A practice library compatible with the different models needs to be developed. This library should include empirical data and equations to simulate the effects of practices on environmental characteristics. Relationships between the parameters of the main methods used to simulate the effects of practices on environmental characteristics will become apparent.
5. Users should only select models that represent catchment structures that are not conservative in the knowledge they may underestimate pesticide transfers.
6. Model structure influences how pesticides are distributed and subjected to transfers processes. Model users and modelers must think carefully about the conceptual environmental compartments needed to simulate the effects of practices together with processes.
7. Semi-distributed models should make it possible for users to enable topological representations of catchments and allow flow interactions and transfers between spatial units. In some place, such interactions might be significant.
8. Natural changes in the vegetated cover of catchment structures (buffer strips, ditches), as well as the effects of management practices on such structures need to be better addressed in catchment models.
9. The results of simulations made with models using the same practice data need to be compared. It is important to check whether (1) pesticide emissions at field borders vary significantly among models, (2) models with better levels of integration of the effects of tillage and mulching better simulate pesticides transfers, and (3) the spatial representation of the organization of the catchment affects contamination by pesticides at the outlet of the catchment. This will highlight the strengths and weaknesses of catchment scale models in assessing the effects of practices on pesticide transfers.

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