# Simulating the effect of techniques and environmental constraints on the spatio-temporal distribution of herbicide applications and stream losses

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Abstract

Technical and environmental constraints on agricultural practices can spatially and temporally concentrate or spread herbicide applications, thereby modifying herbicide losses in stream water. This study analyses the effect of such constraints on spatio-temporal patterns of sowing and weeding activities and, consequently, on herbicide losses, focusing on weeding operations in maize. Machine availability and farmer working time were considered technical constraints, while weather and soil conditions were considered environmental constraints. Simulated experiments were performed with the SACADEAU model, which combines a decision submodel with crop-growth and herbicide-transfer submodels. The decision submodel designed in conjunction with agricultural experts contains decision rules that distribute crop sowing and weeding operations among fields. The model was applied on an agricultural catchment in western Europe, and the results were analysed over nine spring periods. Simulations suggest that, in addition to reducing overall herbicide-application rates, strategies that modify spatial distribution of herbicide applications by reducing herbicide applications in bottomlands could be particularly effective. Temporally distributing herbicide applications, for example via collective machine management, also is effective. Finally, spatial strategies that focus activities on a given area appear to be more efficient than temporal ones that spread activities over time because the former are less dependent on weather conditions.

## 1. Introduction

To reduce the impact of pesticides on human health and ecosystems, the French government introduced the ‘Ecophyto 2018’ plan in 2008. The main objective of this plan is to halve the current use of pesticides in France by promoting agricultural practices that use less of them. Herbicides are a particular concern since they represent one-third of the current pesticide use in France. Maize crops represent 7% of the national surface area and 10% of the current pesticide use, and 75% of the pesticides used on maize are herbicides. In regions with the highest maize production, herbicides represent most of the pesticides detected in rivers (Aubertot et al., 2005). Implementing effective measures to reduce herbicide use and losses is a challenge for agricultural and water management (Campbell et al., 2004).

Many factors affect herbicide stream losses. They can be classified into four categories: (1) site-specific factors - soil and hydrologic properties and geomorphologic characteristics of the catchment; (2) weather factors - particularly precipitation and temperature; (3) anthropogenic factors - land-use and technical management; and (4) herbicide factors - chemical and physical properties and formulation (Lerch and Blanchard, 2003; Müller et al., 2006). These factors have been analysed individually (Müller et al., 2006; Reichenberger et al., 2007; Freitas et al., 2008); however, their interactions rarely have been studied. This diversity of factors demonstrates that mitigating herbicide impacts can involve regulating herbicide amounts or properties, but also involves additional constraints related to their use in space or time based on site-specific, weather, or anthropogenic factors. Such constraints on their use can concentrate or dilute herbicide applications spatially and temporally, thereby influencing herbicide losses. This paper aims to study how such constraints can modify the spatio-temporal distribution of herbicide applications and influence herbicide losses, possibly adding to the mitigating effects of simple reductions in application rates.

Finding answers to this question requires agricultural and environmental impact assessments at the meso-scale (i.e. catchments 10-50 km² in size) to account for high landscape heterogeneity. Agricultural landscapes include farms, which contain a mosaic of fields with various slopes and soils; human infrastructures at field edges, such as grass strips, ditches, or hedgerows; and less-developed areas along streams, such as riparian wetlands. These elements now are known to either buffer or aid in pollutant transport (Colin et al., 2000; Leu et al., 2004a and 2004b). Grass filter strips now are commonly used in regulating herbicide losses at the meso-scale. Therefore, environmental and technical constraints on herbicide applications should consider all of these natural and anthropogenic landscape elements.

Since field experiments are complex (Reichenberger et al., 2007), costly, and sometimes even impossible to perform, particularly at a landscape level, a modelling approach is necessary. The SACADEAU model (French acronym for "Système d'Acquisition des Connaissances pour l'Aide à la Décision sur la qualité de l'eau") is used to test the effect of herbicide application flexibility influenced by environmental and technical constraints (Tortrat, 2004; Trépos, 2008). This model represents biological, physical, and technical processes involved in herbicide applications and their transfer in a catchment. It combines three submodels, the first two previously described by Gascuel-Odoux et al. (2009): a spatially distributed transfer model (SACADEAU-Transf), which represents biochemical and transfer processes in an agricultural landscape, a crop model, and a decision model (SACADEAU-Deci), specifically developed to test the effect of spatial and temporal constraints on herbicide applications. Technical decision processes generally are not considered in herbicide-transfer modelling (Keating and McCown, 2001), and simulation experiments often are based on unique dates, few herbicides, and random spatial and temporal applications (Huber et al., 1998; Du et al., 2006). SACADEAU-Deci fulfils the requirement for representing and analysing effects related both to environmental conditions in a catchment and agricultural constraints on one or more farms, as well as their interactions. In this model, sowing and weeding decisions are made via adaptive sequential plans that have resource and temporal constraints. The model provides agricultural interventions for sowing and weeding (date, location) and herbicide-application characteristics (substance, quantity) according to a set of predefined strategies, including weather and catchment conditions. Spatial constraints of fields are related mainly to their topography and the pattern of agricultural structures, such as farms or groups of farms. Temporal constraints are included, such as rules regarding work-time and agricultural-machine availability. Finally, weather, particularly rainfall, modifies the decision to perform agricultural activities such as sowing and weeding. Consequently, the decision model represents spatial and temporal constraints; therefore, it provides realistic herbicide-application distributions strongly determined by decisions of individual farmers and driven by technical and environmental variables. Consequently, the model predicts their effect on herbicides losses.

This study focuses on simulating maize-crop weeding and herbicide losses to streams in the months following applications to identify factors that could reduce herbicide losses to streams. It addresses two questions: (1) To what extent do technical constraints such as availability of machinery or work time, or environmental constraints such as topographic position influence herbicide losses? (2) Can delineating the location or period of sowing or weeding based on environmental or technical factors further reduce herbicide losses?

## 2. Background

### 2.1. Site and data description

The study site, located in Brittany (in western France), is the 15-km² Frémeur catchment, which has a 28-km-long stream network and a drainage density of 1.65 $km \cdot km^{-2}$ (Fig. 1). The slopes are moderate, with gradients of less than 5%. The landscape is made up of a medium-density bocage (a typical landscape often dedicated to animal production with fields partially surrounded by hedgerows). The soils are silt-loams with a mean organic-matter content around 50 $g \cdot kg^{-1}$. The soil system comprises a well-drained upland and a poorly drained bottomland. The soil overlies weathered bedrock 1-30 m deep that itself overlies fractured Brioverian schist. The physiographic setting is a temperate region with soils displaying moderate to low aggregate stability and shallow groundwater.

This study site is a few kilometres from the Naizin catchment, which has similar physiographic characteristics. This site is highly instrumented and is included in a long-term hydrological observatory (http://www.inra.fr/ore_agrhys) (Molénat et al., 2008) on which some hydrological processes have been studied in detail. The subsurface flow is quantitatively dominant (Molénat et al., 1999 and 2005), and Topmodel already has been applied there successfully (Bruneau et al., 1995; Franks et al., 1998; Molénat et al., 2005). The hypothesis of a water transfer time of more than one year in shallow groundwater of the upper part of the hillslope has been verified (Molénat and Gascuel-Odoux, 2002), as well a rapid and highly variable contamination of the shallow groundwater in the lower part of the hillslope (Molénat and Gascuel-Odoux, 2001). Surface flow occurs during winter as well as spring storm events, when soil surface conditions are degraded (Le Bissonnais et al., 2002). Stream water contamination is due mainly to maize herbicides and occurs in spring (Clément et al., 1999).

A Digital Elevation Model (DEM) of the Frémeur catchment was extracted from an elevation database for Brittany with a resolution of 20 m and was produced by stereoplotting panchromatic SPOT images to a resolution of 10 m. The parcel layer was digitised from the commune's land-registry map on a scale of 1:5000. The drainage network was extracted from the 1:25000 IGN (National Geographic Institute) map and the land-registry map. Field surveys augmented this drainage network by locating ditches, hedges, and grassed filter strips.

Agricultural land accounts for 72% of the total catchment area, the remainder being distributed among woods, wasteland, residential areas, and roads. Agricultural land is distributed as follows: maize (38%), wheat (29%), grassland (21%), and vegetables (5%); the remaining 7% includes fallow land and potatoes. The catchment contains 37 farms, of which 20 measure less than 20 ha. The catchment contains approximately 2000 parcels; in 2000, 1420 were agricultural fields including 148 in maize. Agricultural and maize fields have a mean area of 0.8 ha and 2.7 ha, respectively. This catchment, therefore, exhibits large variability in farm and field size, presenting the complex landscape mosaic common in western Europe.

We selected a 9-year period (1994-2002) to encompass multi-year weather variability. For each year, we focused on 1 Apr - 31 Jul, a period that starts with sowing operations and herbicide applications in maize and finishes when high herbicide concentrations in stream water generally are no longer observed in the field or predicted in herbicide-transfer models. Rainfall during these periods varied moderately (mean ± SD accumulation = 215 ± 80 mm) (Fig. 2, Table 1). The frequency of rain events, characterised by the number of days with rainfall greater than 2 and 10 mm, varied from 14-41 and 2-10, respectively (Table 1). The wettest years were 1994 and 1998, while 1996 was the driest.

Past field observations provided accumulated-discharge data for the 1 Apr - 31 Jul period from 1998-2002. For 1994-1997, daily discharge was simulated by using TopModel (Beven and Kirkby, 1979) (Fig. 2). The application of TopModel to this catchment for studied periods (1 Apr - 31 Jul) for the 7 years where discharge measurements are available (1998-2004), is relevant, as evidenced by Nash Efficiency criterion (Nash and Sutcliffe, 1970) of 0.75. Accumulated discharge calculated for the 1 Apr - 31 Jul period, which mainly depends on the rainfall during the previous months, varied from 0.03 m in 1997 to 0.16 m in 1994 (Table 1).

**2.2. Weed-management practices**

We identified farmers' weed-management practices in the Frémeur catchment from a 2001-2002 survey (Tortrat et al., 2004; Tortrat, 2005). The 75% of farmers for whom pig production was the predominant activity usually followed simple, predefined weeding strategies recommended by technical advisers. We identified three weeding strategies: (i) pre-emergence: a single herbicide application after sowing (the most common); (ii) post-emergence: two herbicide applications at the three- and five- to seven-leaf stages of maize; and (iii) intermediate: two herbicide applications after sowing and at the five-leaf stage. Alternative strategies, such as mechanical or mixed weeding (herbicide on rows and mechanical weeding between rows), were used by 20% of the 37 farmers, who generally shared machinery within cooperative organisations. Such innovative strategies, including a zero or reduced herbicide application rate are already present despite being considered time-consuming and technically difficult compared to a conventional chemical weeding strategy.

The herbicides used depend on the specific weeding strategy. Forty percent of the farmers on this catchment used two herbicides (Merot et al., 2009), having integrated a spatial rationale for herbicide applications: one on bottomlands (at risk for stream contamination) using less mobile and less persistent chemicals and one on uplands using chemicals considered more efficient. Fourteen different chemicals (usually applied at recommended rates) were used on this catchment, highlighting the diversity of technical advisers from agricultural organisations and private or cooperative companies who work in this area.

Herbicide application dates usually remained unknown because farmers often did not record them; thus, only general rules can be provided. Application dates are related to the weeding strategy (pre-emergence or post-emergence) and, therefore, to the stage of maize growth, which is a function of the sowing date and subsequent weather conditions. In the Frémeur catchment, sowing of each field tended to occur either in early April or late April, depending on its slope position. Fields at the bottom of the catchment had hydromorphic soil, experiencing longer periods with wet conditions than soils on the upper slopes. Therefore, to ensure soil workability, sowing and weeding operations generally were delayed on bottomland plots. Weeding operations are generally finished as quickly as possible, in regards to working constraints at the farm scale. Ultimately, herbicide application dates tended to be scattered inside different periods depending on farm and weather constraints. Since 2007, farmers are required to record herbicide application dates, but these data were neither collected nor analysed in this catchment. Hence, such data are absent in the literature, encouraging the use of a decision model to predict them.

This survey revealed that techniques such as reducing the herbicide application rate, adopting spatial or temporal constraints on herbicide application, and increasing collective management of machinery or human work hours already existed in this catchment. Consequently, quantifying the efficiency of such measures and defining measures that could be emphasised to reduce herbicide losses appears relevant.

## 3. The SACADEAU model

### 3.1. Model overview

The SACADEAU simulation model was designed to test the effect of farmers' decisions on stream-water pollution by herbicides. The SACADEAU model combines three submodels that simulate decision-making, crop growth and pollutant transfer (Fig. 3). The latter submodel will be described briefly, as its description was published by Gascuel-Odoux et al. (2009). In contrast, the decision-model is new and therefore presented in detail. Decision-model outputs constitute a portion of inputs to the transfer submodel; in contrast, there is no feedback from the transfer submodel to the decision submodel. Predicted water flows and herbicide concentrations at the catchment outlet depend upon the interaction of all submodels. Furthermore, the SACADEAU model has been included in a meta-modelling framework to identify the main factors influencing water pollution and possible mitigation recommendations, through machine-learning techniques (Cordier, 2005; Cordier et al., 2005; Trépos et al., 2005; Trépos, 2008).

**3.2. Decision submodel**

The decision submodel, designed in conjunction with local agricultural experts, simulates farmers' technical decisions concerning maize crops in the spring, which include the sowing date and weed-management factors (e.g., herbicides used, dates, amounts, locations of herbicide applications) (Fig. 4). As input, the decision submodel uses the spatial distribution of maize crops on the catchment and the corresponding pre-defined sowing and weeding strategies for each of these fields. The submodel then simulates sowing and weeding activities on a daily time-step as a function of weather conditions and technical constraints.

At the field level, the submodel relies on a temporal-window approach that has been used in other decision models, such as Otelo (Aubry et al., 1998), Moderato (Bergez et al., 2002), and Déciblé (Chatelin et al., 2005). This notion of temporal windows, or permitted periods for carrying out an operation, represents the way farmers manage the timing of a crop operation within the overall work organisation on the farm (Chatelin et al., 2005). The beginning and the end of temporal windows for weeding are defined by crop growth predicted by the crop submodel (Fig. 5). When the temporal window for an operation is open, the model checks each field daily to see whether an operation's weather conditions and technical constraints are satisfied. When all conditions are fulfilled, the operation can be performed. We assumed that machine speed, availability of machines and working time, and field area determine the total duration of each operation. When the operation is finished, the operation window closes and simulation continues, waiting for the next operation window to open on the field, until the end of the simulation.

*Temporal windows for sowing and weeding*

In the submodel, the date of sowing influences the development of maize and soil-surface conditions, as well as dynamics of the crop and transfer submodels. For each field, at the beginning of simulation, an early-sowing (10 Apr, day-of-year 100) or late-sowing (1 May, day-of-year 120) date is defined. Weeding operations occur on one or several dates, depending upon the strategy. For example, the window for the pre-emergence strategy opens just after sowing and closes 10 days later (Fig. 5a, Table 2). If weeding cannot be performed during this period, this operation is postponed to a new window that starts at the 3-leaf stage of maize, predicted by the crop submodel (Fig. 5a). Table 2 defines the temporal windows for sowing and the two weeding strategies (pre- and post-emergence). Parameterisation of these temporal windows was based on farmer surveys and the expertise of agricultural advisers. At the time of application, the submodel chooses herbicide types and doses from a database based on each farmer's weeding strategy.

*Environmental and technical conditions*

We assumed that farmers do not sow or apply herbicides on rainy days and that machines cannot work on a field when its soil is too wet to support them. Thus, in the submodel, operations can be performed only if daily rainfall is less than 2 mm and at least 2 days have passed since it last exceeded 2 mm (Table 2). The submodel also contains a daily working-time limit (T) for sowing and weeding operations per farmer. To this limit, overtime ($\varepsilon_T$) can be added to finish an operation on a given field in the same day. We assumed that only one machine performs each operation on a field, at rates of 1 and 4 ha per hour for sowing and weeding, respectively (Table 2).

*Spatial organisation*

The submodel allows organisation of machines at three spatial scales (farm, farm group, and catchment) to determine their use on individual fields. At the individual-farm level, each farm has its own set of machinery and fields that do not change over time (the current scenario of the Frémeur catchment). At the farm-group scale, a farm that has completed its sowing or weeding operations may share machinery with other farms in the group. At the catchment scale, a downhill-slope index (Crave and Gascuel-Odoux, 1997; Merot et al., 2003), slightly modified from the Beven index (Beven and

Kirkby, 1979), is used to classify each field in the catchment as well-drained (uplands) or wet (bottomlands). This index is a good predictor of hydromorphic soils (Merot et al., 2003). Since soil workability is linked to soil water content (Rounsevell et al., 1999) and this latter variable is controlled by topography (Crave and Gascuel-Odoux, 1997), we assumed in the submodels that farmers first work on upland fields of the catchment and then move to bottomlands. The submodel also can use this index to fix the sowing date of each field. Including these three spatial scales in the decision submodel provided the ability to simulate the spatial and temporal distribution of agricultural operations over the catchment in a more realistic manner.

### 3.3. Crop submodel

The only prediction required from the crop submodel is the number of leaves on maize, which determines the starting dates of temporal windows for weeding operations. Leaf number is predicted from cumulative degree days after sowing (Hammer et al., 1993) with a linear equation (i.e., 100, 200, and 300°C to reach 3, 5, and 7 leaves, respectively).

### 3.4. Herbicide-transfer submodel

The transfer model, detailed in Gascuel-Odoux et al. (2009), simulates surface and subsurface flow of herbicide in water, from its application on a field to the outlet of the catchment. The model separately calculates the discharge at the outlet of the catchment and the amount of pesticide transferred by surface and subsurface flow. Here, discharge is considered a global dilution factor affecting the amount of pesticide mobilised in the surface and subsurface flow.

Surface flows of water and pesticide are aggregated at the catchment level using a tree structure linking the plot outlets and their contributing areas. This spatial representation is based on a spatial object-based modelling approach detailed elsewhere (Tortrat and al., 2004; Aurousseau et al., 2009). It allows the upslope surface flow to infiltrate in downslope plots or linear networks. If present, these linear networks, such as hedges or ditches, modify both the flow direction and the location of field outlets, altering this tree structure. According to this spatial model, only 125 of 148 maize fields on the Frémeur catchment were connected to the stream; the other fields were considered total sinks.

Surface flow is controlled either by soil surface sealing on the whole catchment or saturated conditions in bottomlands. The latter is related to the subsurface flow submodel. The surface flow controlled by soil surface sealing is estimated using the concepts and tools developed in the Stream model (Cerdan et al., 2001), an expert-based runoff model using expert rules in the form of matching tables characterising agricultural fields according to soil surface conditions (roughness, soil surface sealing, crop cover) to determine the soil infiltration capacity. This model has been successfully used in a variety of conditions (Evrard et al., 2009).

The subsurface flow model aims to delineate saturated surfaces and estimate the amount of pesticide reaching the groundwater. This is carried out by estimating the storage of pesticide at the soil surface and a transfer coefficient depending on the depth of the water table. The depth of the water table is estimated only on the lower part of the hillslope, since water transfer time in shallow groundwater is estimated to be more than one year for the upper part of the hillslope, which is larger than duration of the studied simulations (4-5 months). Topmodel is used to calculate a mean saturation deficit at each point of the catchment, depending on a topographic index, which can be linked to the water table depth. This submodel provides a daily estimate of the depth of the water table per plot, grouped into different classes over the catchment. Finally, subsurface quantities of herbicide coming from these classes are aggregated into a single reservoir of constant volume that is drained according to a constant drainage coefficient linearly dependent on the catchment's mean water table.

Water and pesticide transfer are coupled in a unique way for the surface and subsurface flow. The initial herbicide concentration in the soil is calculated assuming a complete, rapid, and reversible mixing area between soil and herbicides. Herbicide degradation is predicted using a first-order kinetic equation with a standard half-life parameter. Before each rainfall event, the herbicide quantity in soil is calculated taking into account degradation and surface and subsurface transfer processes since the previous rainfall event. A constant exchange coefficient between soil and water and a fixed area of exchange is used to calculate the herbicide concentration of surface flow. Finally, the amount of herbicide exported by surface and subsurface flow during rainy days is predicted, and the new amount of herbicide stored in soil is calculated. This model has been calibrated on the Frémeur catchment and is partly validated by observations (Gascuel-Odoux et al., 2009).

### 3.5. Model output

The SACADEAU model predicts two variables at the catchment outlet that are spatially and temporally aggregated:

- Weeding Day Accumulation (WDA) is the difference between the last day (*LastWeedingDay*) and the first day (*FirstWeedingDay*) of herbicide application on the entire catchment:

$$\text{WDA} = (\text{LastWeedingDay} - \text{FirstWeedingDay} + 1) \qquad (1)$$

- T-ratio is the ratio of the total amount of herbicides transferred by surface and subsurface routes to the catchment outlet (*herbicide_output*) over the total amount of herbicides applied on the catchment (*herbicide_input*):

$$\text{T-ratio} = \frac{\sum_t \text{herbicide\_ouput}}{\sum_t \text{herbicide\_input}} * 100 \qquad (2)$$

WDA summarises the effect of different environmental and technical constraints on the temporal distribution of weeding operation, while T-ratio summarises the effect of interactions between the spatial and temporal distribution of herbicide applications and the spatial structure of the catchment on the herbicide-transfer rate. Since T-ratio is the output variable of the transfer submodel, the accuracy and robustness of its predictions have been discussed previously (Gascuel-Odoux et al., 2009).

## 4. Simulation experiments

### 4.1. Protocol of simulations

Simulation experiments tested temporal factors related to availability of machines and working time; spatial factors created by the spatial structure of farms, farm groups, or the catchment; and factors related to herbicide dose and proportion of fields treated (Table 3). All simulations were conducted using nine years of weather records (Fig. 2, Table 3). To simplify the interpretation of results, only one weeding strategy (pre-emergence) and one herbicide (dimethenamid) were chosen. We set the properties of dimethenamid, a chloroacetamid, as follows: sorption partition coefficients between water and organic carbon, Koc = 260 cm$^{3.}$.g$^{-1}$·; standard half-life, DT50 = 20 days; application rate of 1.6 L ha$^{-1}$ (active ingredient 1440 g ha$^{-1}$, dimethenamid).

**4.2. Temporal factors: availability of machines and working time**

Experiment 1.1 represented the baseline simulation with no constraints. When conditions allowed working on a field, the operation was performed regardless of the predicted availability of machines or working time. Subsequently, five simulation experiments were performed to study the effect of machine availability (Table 3). Working time was fixed at 8 hours, with a possible overtime of one hour. Each machine was considered as operated by one person, which corresponded to 8 hours of work. For these experiments, an early sowing date was set for fields at higher elevations of the catchment (80% of the fields) and a later date for fields at lower elevations. In experiment 1.2, one machine was allocated per field. In experiment 1.3, one, two or four machines were allocated per farm. In experiment 1.4, one, two or four machines were allocated for the entire catchment (all farms combined). In experiment 1.5, one, two or four machines were allocated for the entire catchment, but machines also managed at farm level. Thus, when a farm's field needed to be worked and a machine was not available on the farm itself, one was allocated if available from the catchment machine pool. This assumption allowed several machines to be allocated to the same farm at the same time. Once the sowing or weeding operation was finished, the machine returned to the catchment pool. Finally, experiment 1.6 was a modification of experiment 1.5 in which the spatial location of fields determined the allocation of machines. When all upland fields (80% of the fields in the catchment) of a farm were sown or weeded, the machine returned to the catchment machine pool.

One experiment was performed to study the effect of farmer working-time (experiment 2.1, Table 3). It considered a maximum working time per day of 4, 6, or 8 hours, with possible overtime of one hour. The minimum working time was set at 4 hours to simulate the fact that farmers do not dedicate all their time to maize-related operations. For these experiments, two dates of sowing and one machine per field were assumed.

### 4.3. Spatio-temporal distribution of sowing operations

Additional simulation experiments tested different sowing dates as a function of the topographic position of fields (Table 3). For these experiments, one machine per field and 8 hours of working time were assumed. Four scenarios were tested: i) all fields with an early sowing date (experiment 3.1); ii) all fields with a late sowing date (experiment 3.2); iii) 80% of the fields with an early sowing date and 20% of the fields with a late sowing date, based on the topographic index as spatial criterion (experiment 3.3); and iv) 150 replicate simulations of random allocations of the late sowing date for 20% of the catchment fields regardless of location to introduce more variability into the previous scenario (experiment 3.4). This last experiment allows us to analyse the effect of different spatial allocation.

### 4.4. Percentage of plots treated and herbicide dose

A final set of five simulation experiments tested different strategies of herbicide reduction, either by reducing the number of fields treated or the herbicide dose (Table 3). For these experiments, two dates of sowing, one machine per field, and 8 hours of working time were assumed. The first experiment varied the percentage of treated fields from 30-100% (experiment 4.1). Then, fixing the percentage of treated fields at 50% (62 plots), we introduced three types of random field selection, performing 150 replicate simulations per year to avoid the effect of specific scenarios on the results. The remaining four experiments simulated ii) random selection among all fields in the catchment (experiment 4.2); iii) random selection of 25 bottomland fields and 37 upland fields using a spatial criterion (experiment 4.3); iv) random selection of 62 upland fields (experiment 4.4); and v) variation in herbicide dose on all plots from 15-100% (experiment 4.5).

## 5. Results

### 5.1. Temporal factors: availability of machines and working time

Depending upon the year, predicted WDA values varied from 2-75 days (Fig. 6a and 6b), while predicted T-ratios varied from 0.1-2.2% among all experiments and years (Fig. 6c and 6d). The low value and variability of predicted T-ratios indicate that a small proportion of herbicides were transferred to the stream, regardless of weather conditions. The highest values of the T-ratio in all experiments corresponded to the two wettest years (1994 and 1998).

Predicted WDA values generally presented the same pattern, marked by low values in 1998, 1999, and 2000 and high values in 1995, 1997, and 2002. The T-ratio and WDA values showed inverse trends: when WDA was short (4 days) the T-ratio was high (1998) and, conversely, when WDA was long (about 25 days), the T-ratio was low (1995-1997, 2001, and 2002). But the variability of the T-ratio cannot simply be explained by a single variable (WDA), as was seen in 2000, when both the predicted WDA and T-Ratio were low (Fig. 6a and 6c).

Three groups of experiments with similar responses could be distinguished regarding WDA. The first corresponded to experiments with any number of machines at the farm or catchment scale, without any consideration of farm relations (experiments 1.1-1.4); among all years, predicted WDA values remained below 20 days (Fig. 6a). The second group corresponded to experiments with only one or two machines per catchment, but considered the spatial constraints of farm structure (experiment 1.5) and catchment topography (experiment 1.6 with 2 machines per catchment), for which predicted WDA varied among years from 40-75 days (Fig. 6b). The third group assuming four machines available with the same constraints (experiments 1.5 and 1.6) presented intermediate results (Fig. 6b). The values of the T-ratio could not be split clearly between these groups because of different trends from year to year. Therefore, the effect of machine availability on the T-ratio initially depended on the year. This was particularly well observed in experiment 1.5, with one machine available for the entire catchment. In this case, the T-ratio was either the lowest (1994, 1996, 1998, and 2002) or the highest (1995, 1997, 1999, and 2000) (Fig. 6d). Moreover collective machine management at the catchment scale that also considers the farm scale may reduce herbicide transfer significantly during some years by temporarily increasing in time the distribution of weeding operations like in 1994 (Fig. 6b and 6d).

The availability of working time as tested here (experiment 2.1) had no effect on predicted WDA or T-ratio values, which were similar to those in the baseline (experiment 1.1). Working time did not constrain the spatial distribution of weeding operations and therefore had no effect on the T-ratio.

**5.2. Spatio-temporal distribution of sowing operations**

Predicted WDA was short for both early and late sowing (Fig. 7a). As expected, a scenario with 80% early sowing and 20% late sowing (experiment 3.3) greatly extend this duration. However, this experiment did not give the lowest T-ratio.

The effect of the sowing date on the T-ratio also depended on the year (Fig. 7a). From 1997-2000, this factor has no effect on the T-ratio, whereas the effect was large for 1994, 2001, and 2002. Early sowing for all fields (experiment 3.1) gave the lowest T-ratio, except for 2001. The results for the scenario with 80% early sowing and 20% late sowing (experiment 3.3) provided a little higher T-ratio than the experiment 3.1. Considering this latest scenario (experiment 3.3), the results were relatively similar when date of sowing of fields were selected randomly (experiment 3.4) (Fig. 7b), except in 1994 and 2002 for which T-ratio was lower, and 2001 for which it was higher. These results show that considering different sowing dates, with (Fig. 7a) or without spatial criteria (Fig. 7b), did not consistently lead to a lower T-ratio except for a particularly rainy year like 1994 when early sowing can be promoted.

**5.3. Percentage and allocation of fields treated and herbicide dose**

The T-ratio decreased as the number of weeded fields decreased for all years (experiment 4.1), except in 1997, when it was always near zero. The range of the decrease depends on the year (Fig. 8a). It decreased from 2 to 0.6% and from 1.5 to 0.7%, in 1994 and 1998, respectively (Fig. 8a). A slight decrease in the percentage of fields weeded from 100 to 90% led to a significant decrease of the T-ratio, particularly when the T-ratio was high, as in 1994. Lastly, reducing the percentage of fields weeded decreased the T-ratio more than reducing the application rate (Fig. 8a). Indeed, the results of experiment 4.1 with 100 % of fields weeded were similar to those of experiment 4.5, regardless of the herbicide dose. In comparison to experiment 4.2, when a larger percentage of treated fields were randomly selected from bottomland (experiment 4.3), T-ratio increased (Figs. 8b and 8c). When herbicide applications were limited to upland fields (experiment 4.4), predicted T-ratios were lower than 1% (Fig. 8d), and the range of variation was lower than those of the other two spatial scenarios (Figs. 8b and 8c).

## 6. Discussion

### 6.1. Utility, evaluation and improvement of the model

Developing and combining a decision model with crop and transfer models constitutes the uniqueness of this modelling approach; it shows that herbicide stream-water contamination is the result of a conjunction of environmental conditions, such as weather and soil patterns, and technical constraints, such as machine availability.

The relevance of a model comes from the innovative measures that it can suggest or from the support it can provide to stakeholders regarding mitigation measures. From this point of view, we can emphasise the unexpected effect of machine availability on predicted herbicide losses in our simulations, which requires further investigation. We also highlight the comparison of the effects of different herbicide-reduction strategies, which suggest the potential for reducing herbicide losses by implementing spatial constraints on herbicide applications.

The validation of such a model from observations is challenging. A rigorous validation process would require detailed data on the spatial and temporal distribution of the quantities of herbicides applied over the catchment. These data are not available at the present time, especially not for a long time-series, but they should be in the future, now that recent regulations require recording quantities of herbicide applied. In contrast, the elaboration of the model and the distribution of simulated sowing and weeding dates were discussed with local agricultural experts, who deemed them coherent.

A sensitivity analysis of the parameters was performed on the allocation of sowing and weeding dates. The number of replicate simulations (150 per year) (Fig. 7b and 8b,c,d) and the length of the weather series (nine years) covers a large range of environmental and technical conditions and yielded a predicted T-ratio that ranged from 0.1-3.5%. The observed T-ratio ranges from 0.1 to 0.6 % for six years (Clément et al., 1999) and therefore is included in the range of simulated T-ratio. The larger range of T-ratio is explained by a larger range of simulated conditions. Predictions were made assuming an average herbicide decay-rate (DT50), but it would be useful to test a wider range of values of this property, since they may influence herbicide losses greatly. Further experiments could also be done to test the effect of spatial and temporal distribution of agricultural activities. Especially, the spatial rule 'farmers first work on upland fields of the catchment, then move to bottomlands' could be relaxed or changed by analyzing its effects on T-ratio and WDA values. This rule is adapted to the studied environmental conditions where the bottom lands are longer wet than uplands, but could be relaxed in other environmental conditions.

The model could be improved by including other processes such as the pre-sowing operations of ploughing or seed-bed preparation. These pre-sowing operations will influence the timing of operations that follow, depending on soil type and weather (Leenhardt and Lemaire, 2002), and influence water infiltration and surface runoff. Also, strategies based on observations of weed encroachment could be taken into account to adapt weeding operations. This improvement would require a crop model that represents weed growth and crop-weed competition. Adding equations to quantify yield effects of the different strategies also could help test their acceptability to farmers. Functions to adapt the herbicide dose to weather conditions also could be added. Because of the modular structure of SACADEAU, it has few limits to the inclusion and the test of different or more sophisticated models. Lastly, the output variables studied could be improved, in particular WDA, which describes the duration of weeding operations but not the effective number of working days for weeding or the spatial distribution of weeding operations. To estimate spatial distribution, an equation that calculates the mean distance of weeded plots to the stream over time could be proposed.

**6.2. Interactions between agricultural practices and weather conditions**

The effect of weather on the WDA and the T-ratio is obvious but complex due to interactions between weather conditions and the spatial distribution of sowing and weeding operations. The effect of rainfall amount and frequency during each year is high. For the rainiest years of 1994 and 1998, the T-ratio and its variability are highest due to large individual rainfall events and rainfall frequency.

The date of one rainfall event can have a large effect on the WDA and the T-ratio. For example, in the case of machine availability experiments, in simulation experiment 1.6 in 1998 (a rainy year), the WDA with one machine per catchment had a lower predicted WDA (18 days, days-of-year 150-167) than that with two machines per catchment (65 days, days-of-year 103-167). Having one fewer machine on the catchment moved sowing dates to a rainier period in which pre-emergence weeding became impossible, delaying the entire weeding program to the 3-leaf stage.

The distribution of rain also could have a significant effect on the WDA and the T-ratio, as shown when comparing the results experiments 3.1 (early sowing) and 3.2 (late sowing) in the two rainiest years (1994 and 1998). The predicted early-sowing T-ratio was half that of the late-sowing T-ratio in 1994 but not in 1998 (Fig. 7a), despite similar rainfall amounts (Table 2). Analysis of the simulations shows that rainfall events in early spring 1998 concentrated weeding operations around day-of-year 122 regardless of the sowing date. Conversely, the absence of rainfall in early spring 1994 separated weeding operations into two periods according to the sowing strategy. Consequently, in 1994 predicted herbicide concentrations in the soil were lower after early sowing than late sowing because they had approximately 20 additional days to degrade. The low predicted T-ratio for the early sowing date in all 9 years shows that this date best limited herbicide transfer; however, this effect can be modified by spring rainfall distribution.

Weather factors had smaller effects on the T-ratio, with low intra- and inter-year variability when herbicide applications were located on upland fields (Fig. 8d). Analysis of the relation between predicted WDA and T-ratio for all experiments and all years (Fig. 9) shows that these variables were partially correlated in years of exceptional rainfall (1994 and 1998). In 1998, T-ratio increased as

WDA increased, whereas in 1994, for WDA higher than 40 days, T-ratio decreased as WDA increased (Fig. 9). In other years, the predicted T-ratio ranged from 0.2-1% regardless of WDA.

Finally, rainfall can delay herbicide applications, temporally concentrating them on a catchment, and increase herbicide transfer to streams by increasing runoff; both of these rainfall effects can increase the herbicide transfer ratio. A better investigation of the influence of rainfall could be achieved by using simulated weather in the model that specifies rainfall amount and frequencies, and by improving modelling at short timescale. The surface runoff model operates at hourly timescale, which does not allow the model to simulate correctly runoff and herbicide transfer when short and intense rainfall events occur at minutes to few hours scale. Not taking such flushing events into account may lead to underestimate the water and herbicide transfer.

### 6.3. Strategies to reduce herbicide pollution

Despite strong interactions between agricultural activities and weather conditions, and high inter-annual variability of T-ratio, which weeding strategies can be recommended? The results of the numeric experiments have been aggregated over the nine chosen years to compare them (Fig. 10). An experiment is more effective as the median and the variability are low, i.e. effective whatever the climatic conditions. From this criterion, experiments which reduce proportion of plots treated (experiment 4.1), especially by avoiding herbicide application bottomland fields of the catchment (experiment 4.4), are particularly effective. This mitigation measure must be undertaken collectively at the catchment scale because it would not imply the same constraints on all farms.

Among all experiments, variations in working time had no effect because the 4-hours minimum was sufficient to perform the operations due to small size and low number of plots per farm, small farms sizes and high machine-throughput rates. As this variable seems to be context dependant, the application of the model to other contexts (larger plots, more plots, and more farms) could be interesting especially to test the sensitivity of this variable to the context, and analyze the effect of higher up to extreme of working time when conditions are optimal for farmers.

Similarly, machine management simultaneously at the farm and catchment scales always was sufficient to apply herbicide to all catchment fields (Fig. 6). As for the T-ratio, we can say that working time and machine availability are often over-dimensioned in simulations. A simulation considering that only 1-2 machines per catchment were able to distribute weeding operations over time and halve the T-ratio from 2.2 to 1% in 1994 and 1.6 to 0.8% in 1998 (experiment 1.5, Fig. 6d). Collective machine management and constraints on machine availability could be considered as potential factors to reduce water contamination at this stage of an exploratory approach. These scenarios would have to be tested with a more complex crop model to evaluate the effects of such measures on crop development, yield, and weed management and evaluate their acceptability by farmers and to analyse the variability regarding climatic conditions.

## 7. Conclusion

The decision submodel was developed to simulate decisions of farmers for sowing and weeding activities that take into account environmental constraints such as weather and slope position of the plots and technical constraints such as the availability of machines and farmers' working time. These operations are performed during temporal windows if certain conditions are fulfilled. The decision submodel distributes a given agricultural operation over time and space more realistically than random or unique methods commonly used in numerical simulations.

Simulation results show that herbicide transfer is not only the effect of the quantity of herbicides applied, but of technical and environmental factors that interact to concentrate or spread herbicide applications over time and space. Herbicide transfer depends greatly on annual weather conditions. Collective machine management and an early sowing date can decrease herbicide transfer, but their effects vary according to weather conditions. Nonetheless, these practices could be promoted more frequently. Spatial strategies that decrease the number of fields in the catchment on which herbicides are applied are always effective, particularly when herbicide applications occur only on upland fields.

Finally, our simulations indicate that modifying the spatio-temporal distribution of herbicide applications by considering environmental and technical constraints does not automatically decrease herbicide transfer rates, as assumed. The effect of a higher flexibility in time and space in herbicide applications appears to depend strongly on weather conditions, generally becoming more effective during rainy years.

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**Figure captions**

Figure 1. Location of the Frémeur catchment in western France and land use of its 2000 parcels.

Figure 2. Rainfall (mm/day) and discharge (m/day) on the study catchment from 1 Apr to 31 Jul for 1994-2002. The vertical dotted line shows the temporal discontinuity between periods.

Figure 3. General SACADEAU model diagram. The T-ratio equals the ratio between predicted herbicide output and input. WDA (Weeding Day Accumulation) equals the difference between the last and first days of herbicide application on the catchment.

Figure 4. Decision-model diagram. $\varepsilon_{Rainfall}$ = rainfall threshold; $t_{RainfallEvent}$ = day with rainfall higher than $\varepsilon_{Rainfall}$

Figure 5. Temporal diagram of decisions for (a) pre-emergence and (b) post-emergence weeding strategies. Plain brackets correspond to fixed dates and dotted brackets correspond to simulated variable dates.

Figure 6. Predicted T-ratio and WDA from 1994-2002 for simulation experiments 1.1 to 1.6. (mach = machine). The legend of graph (c) is used for graph (a) and the legend of graph (d) is used for graph (b). See Table 3 for simulation experiments abbreviations.

Figure 7. a) predicted T-ratio and WDA from 1994-2002 for simulation experiment 3.1-3.3 (3.1: all fields have an early sowing date; 3.2: all fields have a late sowing date; 3.3: 80% of fields have an early sowing date and 20% a late date); b) predicted T-ratio from 1994-2002 for simulation experiments 3.3 and 3.4. Standard boxplots show variability of predicted T-ratio from experiment 3.4. See Table 3 for simulation experiments abbreviations.

Figure 8. a) predicted T-ratio from 1994-2002 when the percentage of weeded fields decreased (experiment 4.1). Standard boxplots of predicted T-ratio from 1994-2002 with 50% of fields treated with b) random choice from all fields (experiment 4.2); c) random choice of 25 bottomland fields and 37 upland fields (experiment 4.3); d) random choice of 62 upland fields (experiment 4.4). See Table 3 for simulation experiments abbreviations.

Figure 9. Comparison of predicted WDA (Weeding Day Accumulation) and T-ratio for all simulation experiments by year.

Figure 10. Standard boxplots of predicted T-ratio for all experiments with all years aggregated.  See Table 3 for simulation experiments abbreviations.