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1 Simulating the effect of technical and environmental constraints on the spatio-temporal
2 distribution of herbicide applications and stream losses

3

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25 Abstract

26

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

43 **1. Introduction**

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

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

66 Finding answers to this question requires agricultural and environmental impact assessments at
67 the meso-scale (i.e. catchments 10-50 km² in size) to account for high landscape heterogeneity.
68 Agricultural landscapes include farms, which contain a mosaic of fields with various slopes and soils;
69 human infrastructures at field edges, such as grass strips, ditches, or hedgerows; and less-developed

70 areas along streams, such as riparian wetlands. These elements now are known to either buffer or aid
71 in pollutant transport (Colin et al., 2000; Leu et al., 2004a and 2004b). Grass filter strips now are
72 commonly used in regulating herbicide losses at the meso-scale. Therefore, environmental and
73 technical constraints on herbicide applications should consider all of these natural and anthropogenic
74 landscape elements.

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

97 perform agricultural activities such as sowing and weeding. Consequently, the decision model
98 represents spatial and temporal constraints; therefore, it provides realistic herbicide-application
99 distributions strongly determined by decisions of individual farmers and driven by technical and
100 environmental variables. Consequently, the model predicts their effect on herbicides losses.

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

107

108 **2. Background**

109 **2.1. Site and data description**

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

118 This study site is a few kilometres from the Naizin catchment, which has similar physiographic
119 characteristics. This site is highly instrumented and is included in a long-term hydrological
120 observatory (http://www.inra.fr/ore_agrhys) (Molénat et al., 2008) on which some hydrological
121 processes have been studied in detail. The subsurface flow is quantitatively dominant (Molénat et al.,
122 1999 and 2005), and Topmodel already has been applied there successfully (Bruneau et al., 1995;
123 Franks et al., 1998; Molénat et al., 2005). The hypothesis of a water transfer time of more than one

124 year in shallow groundwater of the upper part of the hillslope has been verified (Molénat and Gascuel-
125 Odoux, 2002), as well a rapid and highly variable contamination of the shallow groundwater in the
126 lower part of the hillslope (Molénat and Gascuel-Odoux, 2001). Surface flow occurs during winter as
127 well as spring storm events, when soil surface conditions are degraded (Le Bissonnais et al., 2002).
128 Stream water contamination is due mainly to maize herbicides and occurs in spring (Clément et al.,
129 1999).

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

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

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

151 Past field observations provided accumulated-discharge data for the 1 Apr - 31 Jul period from 1998-
152 2002. For 1994-1997, daily discharge was simulated by using TopModel (Beven and Kirkby, 1979)
153 (Fig. 2). The application of TopModel to this catchment for studied periods (1 Apr - 31 Jul) for the 7
154 years where discharge measurements are available (1998-2004), is relevant, as evidenced by Nash
155 Efficiency criterion (Nash and Sutcliffe, 1970) of 0.75. Accumulated discharge calculated for the 1
156 Apr - 31 Jul period, which mainly depends on the rainfall during the previous months, varied from
157 0.03 m in 1997 to 0.16 m in 1994 (Table 1).

158

159 **2.2. Weed-management practices**

160 We identified farmers' weed-management practices in the Frémeur catchment from a 2001-
161 2002 survey (Tortrat et al., 2004; Tortrat, 2005). The 75% of farmers for whom pig production was the
162 predominant activity usually followed simple, predefined weeding strategies recommended by
163 technical advisers. We identified three weeding strategies: (i) pre-emergence: a single herbicide
164 application after sowing (the most common); (ii) post-emergence: two herbicide applications at the
165 three- and five- to seven-leaf stages of maize; and (iii) intermediate: two herbicide applications after
166 sowing and at the five-leaf stage. Alternative strategies, such as mechanical or mixed weeding
167 (herbicide on rows and mechanical weeding between rows), were used by 20% of the 37 farmers, who
168 generally shared machinery within cooperative organisations. Such innovative strategies, including a
169 zero or reduced herbicide application rate are already present despite being considered time-
170 consuming and technically difficult compared to a conventional chemical weeding strategy.

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

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

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

196

197

198 **3. The SACADEAU model**

199 **3.1. Model overview**

200 The SACADEAU simulation model was designed to test the effect of farmers' decisions on
201 stream-water pollution by herbicides. The SACADEAU model combines three submodels that
202 simulate decision-making, crop growth and pollutant transfer (Fig. 3). The latter submodel will be
203 described briefly, as its description was published by Gascuel-Oudoux et al. (2009). In contrast, the
204 decision-model is new and therefore presented in detail. Decision-model outputs constitute a portion

205 of inputs to the transfer submodel; in contrast, there is no feedback from the transfer submodel to the
206 decision submodel. Predicted water flows and herbicide concentrations at the catchment outlet depend
207 upon the interaction of all submodels. Furthermore, the SACADEAU model has been included in a
208 meta-modelling framework to identify the main factors influencing water pollution and possible
209 mitigation recommendations, through machine-learning techniques (Cordier, 2005; Cordier et al.,
210 2005; Trépos et al., 2005; Trépos, 2008).

211

212 **3.2. Decision submodel**

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

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

232 *Temporal windows for sowing and weeding*

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

244 *Environmental and technical conditions*

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

252 *Spatial organisation*

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

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

267

268 **3.3. Crop submodel**

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

273

274 **3.4. Herbicide-transfer submodel**

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

280 Surface flows of water and pesticide are aggregated at the catchment level using a tree structure
281 linking the plot outlets and their contributing areas. This spatial representation is based on a spatial
282 object-based modelling approach detailed elsewhere (Tortrat and al., 2004; Arousseau et al., 2009). It
283 allows the upslope surface flow to infiltrate in downslope plots or linear networks. If present, these
284 linear networks, such as hedges or ditches, modify both the flow direction and the location of field

285 outlets, altering this tree structure. According to this spatial model, only 125 of 148 maize fields on the
286 Frémeur catchment were connected to the stream; the other fields were considered total sinks.

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

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

305 Water and pesticide transfer are coupled in a unique way for the surface and subsurface flow. The
306 initial herbicide concentration in the soil is calculated assuming a complete, rapid, and reversible
307 mixing area between soil and herbicides. Herbicide degradation is predicted using a first-order kinetic
308 equation with a standard half-life parameter. Before each rainfall event, the herbicide quantity in soil
309 is calculated taking into account degradation and surface and subsurface transfer processes since the
310 previous rainfall event. A constant exchange coefficient between soil and water and a fixed area of
311 exchange is used to calculate the herbicide concentration of surface flow. Finally, the amount of

312 herbicide exported by surface and subsurface flow during rainy days is predicted, and the new amount
313 of herbicide stored in soil is calculated. This model has been calibrated on the Frémeur catchment and
314 is partly validated by observations (Gascuel-Oudoux et al., 2009).

315

316 **3.5. Model output**

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

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

$$321 \quad \text{WDA} = (\text{LastWeedingDay} - \text{FirstWeedingDay} + 1) \quad (1)$$

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

$$325 \quad \text{T-ratio} = \frac{\sum_t \text{herbicide_output}}{\sum_t \text{herbicide_input}} * 100 \quad (2)$$

326 WDA summarises the effect of different environmental and technical constraints on the
327 temporal distribution of weeding operation, while T-ratio summarises the effect of interactions
328 between the spatial and temporal distribution of herbicide applications and the spatial structure of the
329 catchment on the herbicide-transfer rate. Since T-ratio is the output variable of the transfer submodel,
330 the accuracy and robustness of its predictions have been discussed previously (Gascuel-Oudoux et al.,
331 2009).

332

333 **4. Simulation experiments**

334 **4.1. Protocol of simulations**

335 Simulation experiments tested temporal factors related to availability of machines and working
336 time; spatial factors created by the spatial structure of farms, farm groups, or the catchment; and
337 factors related to herbicide dose and proportion of fields treated (Table 3). All simulations were

338 conducted using nine years of weather records (Fig. 2, Table 3). To simplify the interpretation of
339 results, only one weeding strategy (pre-emergence) and one herbicide (dimethenamid) were chosen.
340 We set the properties of dimethenamid, a chloroacetamid, as follows: sorption partition coefficients
341 between water and organic carbon, $K_{oc} = 260 \text{ cm}^3 \cdot \text{g}^{-1}$; standard half-life, $DT_{50} = 20$ days;
342 application rate of 1.6 L ha^{-1} (active ingredient 1440 g ha^{-1} , dimethenamid).

343

344 **4.2. Temporal factors: availability of machines and working time**

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

362 One experiment was performed to study the effect of farmer working-time (experiment 2.1,
363 Table 3). It considered a maximum working time per day of 4, 6, or 8 hours, with possible overtime of
364 one hour. The minimum working time was set at 4 hours to simulate the fact that farmers do not

365 dedicate all their time to maize-related operations. For these experiments, two dates of sowing and one
366 machine per field were assumed.

367

368 **4.3. Spatio-temporal distribution of sowing operations**

369 Additional simulation experiments tested different sowing dates as a function of the topographic
370 position of fields (Table 3). For these experiments, one machine per field and 8 hours of working time
371 were assumed. Four scenarios were tested: i) all fields with an early sowing date (experiment 3.1); ii)
372 all fields with a late sowing date (experiment 3.2); iii) 80% of the fields with an early sowing date and
373 20% of the fields with a late sowing date, based on the topographic index as spatial criterion
374 (experiment 3.3); and iv) 150 replicate simulations of random allocations of the late sowing date for
375 20% of the catchment fields regardless of location to introduce more variability into the previous
376 scenario (experiment 3.4). This last experiment allows us to analyse the effect of different spatial
377 allocation.

378

379 **4.4. Percentage of plots treated and herbicide dose**

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

390

391

392 5. Results

393 5.1. Temporal factors: availability of machines and working time

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

399 Predicted WDA values generally presented the same pattern, marked by low values in 1998,
400 1999, and 2000 and high values in 1995, 1997, and 2002. The T-ratio and WDA values showed
401 inverse trends: when WDA was short (4 days) the T-ratio was high (1998) and, conversely, when
402 WDA was long (about 25 days), the T-ratio was low (1995-1997, 2001, and 2002). But the variability
403 of the T-ratio cannot simply be explained by a single variable (WDA), as was seen in 2000, when both
404 the predicted WDA and T-Ratio were low (Fig. 6a and 6c).

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

419 some years by temporarily increasing in time the distribution of weeding operations like in 1994 (Fig.
420 6b and 6d).

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

425

426 **5.2. Spatio-temporal distribution of sowing operations**

427 Predicted WDA was short for both early and late sowing (Fig. 7a). As expected, a scenario with
428 80% early sowing and 20% late sowing (experiment 3.3) greatly extend this duration. However, this
429 experiment did not give the lowest T-ratio.

430 The effect of the sowing date on the T-ratio also depended on the year (Fig. 7a). From 1997-
431 2000, this factor has no effect on the T-ratio, whereas the effect was large for 1994, 2001, and 2002.
432 Early sowing for all fields (experiment 3.1) gave the lowest T-ratio, except for 2001. The results for
433 the scenario with 80% early sowing and 20% late sowing (experiment 3.3) provided a little higher T-
434 ratio than the experiment 3.1. Considering this latest scenario (experiment 3.3), the results were
435 relatively similar when date of sowing of fields were selected randomly (experiment 3.4) (Fig. 7b),
436 except in 1994 and 2002 for which T-ratio was lower, and 2001 for which it was higher. These results
437 show that considering different sowing dates, with (Fig. 7a) or without spatial criteria (Fig. 7b), did
438 not consistently lead to a lower T-ratio except for a particularly rainy year like 1994 when early
439 sowing can be promoted.

440

441 **5.3. Percentage and allocation of fields treated and herbicide dose**

442 The T-ratio decreased as the number of weeded fields decreased for all years (experiment 4.1),
443 except in 1997, when it was always near zero. The range of the decrease depends on the year (Fig. 8a).
444 It decreased from 2 to 0.6% and from 1.5 to 0.7%, in 1994 and 1998, respectively (Fig. 8a). A slight
445 decrease in the percentage of fields weeded from 100 to 90% led to a significant decrease of the T-

446 ratio, particularly when the T-ratio was high, as in 1994. Lastly, reducing the percentage of fields
447 weeded decreased the T-ratio more than reducing the application rate (Fig. 8a). Indeed, the results of
448 experiment 4.1 with 100 % of fields weeded were similar to those of experiment 4.5, regardless of the
449 herbicide dose. In comparison to experiment 4.2, when a larger percentage of treated fields were
450 randomly selected from bottomland (experiment 4.3), T-ratio increased (Figs. 8b and 8c). When
451 herbicide applications were limited to upland fields (experiment 4.4), predicted T-ratios were lower
452 than 1% (Fig. 8d), and the range of variation was lower than those of the other two spatial scenarios
453 (Figs. 8b and 8c).

454

455 **6. Discussion**

456 **6.1. Utility, evaluation and improvement of the model**

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

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

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

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

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

499

500 **6.2. Interactions between agricultural practices and weather conditions**

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

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

511 The distribution of rain also could have a significant effect on the WDA and the T-ratio, as
512 shown when comparing the results experiments 3.1 (early sowing) and 3.2 (late sowing) in the two
513 rainiest years (1994 and 1998). The predicted early-sowing T-ratio was half that of the late-sowing T-
514 ratio in 1994 but not in 1998 (Fig. 7a), despite similar rainfall amounts (Table 2). Analysis of the
515 simulations shows that rainfall events in early spring 1998 concentrated weeding operations around
516 day-of-year 122 regardless of the sowing date. Conversely, the absence of rainfall in early spring 1994
517 separated weeding operations into two periods according to the sowing strategy. Consequently, in
518 1994 predicted herbicide concentrations in the soil were lower after early sowing than late sowing
519 because they had approximately 20 additional days to degrade. The low predicted T-ratio for the early
520 sowing date in all 9 years shows that this date best limited herbicide transfer; however, this effect can
521 be modified by spring rainfall distribution.

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

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

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

536

537 **6.3. Strategies to reduce herbicide pollution**

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

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

552 Similarly, machine management simultaneously at the farm and catchment scales always was
553 sufficient to apply herbicide to all catchment fields (Fig. 6). As for the T-ratio, we can say that
554 working time and machine availability are often over-dimensioned in simulations. A simulation
555 considering that only 1-2 machines per catchment were able to distribute weeding operations over time
556 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).
557 Collective machine management and constraints on machine availability could be considered as
558 potential factors to reduce water contamination at this stage of an exploratory approach. These
559 scenarios would have to be tested with a more complex crop model to evaluate the effects of such
560 measures on crop development, yield, and weed management and evaluate their acceptability by
561 farmers and to analyse the variability regarding climatic conditions.

562

563

564 **7. Conclusion**

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

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

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

583

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710 **Figure captions**

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

712 Figure 2. Rainfall (mm/day) and discharge (m/day) on the study catchment from 1 Apr to 31 Jul for
713 1994-2002. The vertical dotted line shows the temporal discontinuity between periods.

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

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

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

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

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

730 Figure 8. a) predicted T-ratio from 1994-2002 when the percentage of weeded fields decreased
731 (experiment 4.1). Standard boxplots of predicted T-ratio from 1994-2002 with 50% of fields treated
732 with b) random choice from all fields (experiment 4.2); c) random choice of 25 bottomland fields and
733 37 upland fields (experiment 4.3); d) random choice of 62 upland fields (experiment 4.4).

734 See Table 3 for simulation experiments abbreviations.

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

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