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1 **PESTIPOND: A descriptive model of pesticide fate in artificial**

2 **ponds: II. Model application and evaluation**

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13 **Abstract**

14 Some artificial ponds (APs) are designed to collect part of the agricultural water fluxes and
15 dissipate their pesticide contamination through a synergy of physicochemical processes. APs
16 act as buffer zones and mitigate pesticide transfer of farm plots to natural water resources. As
17 part of a two-paper series, this paper addresses the application and validation of the
18 PESTIPOND model. PESTIPOND is a process-based model developed to predict pesticides'
19 behavior and distribution in APs located in drained agricultural catchments. The development
20 and sensitivity analysis of the model are described in Paper I ([Bahi et al., 2023a](#)). PESTIPOND
21 was applied on the Rampillon AP to characterize the fate of seven different pesticides and five
22 monitoring periods while considering the key transfer and transformation processes. The model
23 was assessed through various methods against the observed data in simulating pesticide
24 dynamics. The statistical and graphical evaluation of PESTIPOND reflected a good
25 performance except for boscalid. The sensitivity analysis and application of the model
26 evidenced that adsorption-desorption and biotransformation in the pond water are major
27 processes behind pesticide dissipation. Hydrophobic and lowly mobile pesticides are more
28 likely to be bio-transformed at the water-sediment interface. This work highlights the link
29 between the hydraulic residential time (HRT), temperature, and APs' efficiency in minimizing
30 pesticide transfer into the environment. The model predicted that the actual efficiency of the
31 AP covering 0.15% of the drained catchment would double if the pond's surface area covered
32 at least 1% of the catchment. Moreover, the model's predictions evidenced that a temperature
33 rise of 10°C will increase the dissipation of pesticides by only 8%. PESTIPOND provides key
34 elements that are useful to design and manage ponds with optimal efficiency. Hence, these APs
35 can be complementary solutions to pesticide use regulation to reduce the transfer of agricultural
36 contamination into freshwater resources.

37 **Keywords:**

38 Pesticide; artificial pond; model; mass budget; dissipation; calibration

39 **1 Introduction**

40 Due to the broad-spectrum toxicity of pesticides, they are a non-point source of pollution for
41 the ecosystem since they are transferred from agricultural plots to natural water resources
42 through surface runoff and subsurface drainage. Pesticides are particularly pernicious for the
43 ecosystem compared to other chemicals because they are specially manufactured to eliminate pests
44 (Ippolito et al., 2015). As such, pesticides are a major risk for terrestrial and aquatic biodiversity
45 (Messelink et al., 2021; Mineau and Whiteside, 2013) and the ecosystem's functioning (Brühl and
46 Zaller, 2021). There is now compelling evidence that certain pesticides exhibit a serious hazard to
47 humans and other life forms, as well as undesired side effects on the environment (Briggs, 2018;
48 Edwards, 2013; Nagy et al., 2020).

49 Hence, the need to reduce pesticide inputs into water resources, as they are substantial drinking
50 water supplies and aquatic habitats (Leenhardt et al., 2022). Pesticides have been detected in
51 groundwater (Baran et al., 2008; Hunter, 2012), rivers (Montiel-León et al., 2019; Xu et al.,
52 2020), and lakes (Bhardwaj et al., 2019; Kandie et al., 2020), as well as smaller wetlands
53 (Lorenz et al., 2017; Ulrich et al., 2018), making pesticides a major cause for water quality
54 impairment. As complements to pesticide use regulation and management practices, material
55 solutions can be implemented to safeguard the quality of water resources and mitigate pesticide
56 input into water bodies, such as edge-of-field and riparian buffer strips, vegetated ditches,
57 wetlands, and artificial ponds (Vymazal and Brezinova, 2015).

58 This study focuses on constructed wetlands, especially edge-of-field artificial ponds (APs)
59 since they have the advantages of needing minimal operations and providing wildlife habitat
60 (Sudarsan and Nithiyantham, 2021). APs are also known for their cost-effectiveness and low
61 energy consumption compared to other surface water treatment methods (e.g., coagulation,
62 membrane filtration, ion exchange, photocatalytic degradation, and adsorption on black carbon
63 and activated carbon) (Aungpradit et al., 2007; Fitch, 2014; Kearns et al., 2014; Trepel, 2010).
64 In practice, edge-of-field APs can act as buffer zones since they are constructed downstream
65 agricultural plots and upstream natural water resources. APs can intercept a part of agricultural
66 water, and after important flow events, the water leaving APs can be less pesticide-loaded, and
67 contamination transfer into the environment can be dissipated. Over the past years and in light
68 of the worsening water shortage, the evaluation of APs environmental role has gained
69 significant attention. The efficiency of APs in reducing pesticide transfer into the environment
70 was widely reiterated in literature (Li et al., 2014; Tournebize et al., 2017; Vymazal and
71 Brezinova, 2015; Zhang et al., 2014). APs provide an area for a series of physicochemical
72 processes to dissipate pesticide water contamination.

73 Modeling is a practical tool to assess the performance of APs and explore the physicochemical
74 processes behind pesticide dissipation in APs. Modeling can be used to improve the efficiency
75 of APs to safeguard water quality. Models of varying levels of complexity have been developed
76 and applied to field data to gain insight into the performance of APs. However, many of these
77 models were dedicated to simulating nutrient behavior (Kalin et al., 2013; Son et al., 2010;
78 Sonavane and Munavalli, 2009), and fewer models were assigned to pesticides. Among
79 pesticide fate models are the risk assessment models such as PRZM (Carsel, 1998) and
80 MACRO (Larsbo and Jarvis, 2003; Larsbo et al., 2005), which simulate pesticide fate in the
81 root zone and macro-porous field soils, respectively, and TOXSWA (Adriaanse, 1996) from
82 the FOCUS group (Tooby, 1999), to model pesticide fate in ditches. These models provide

83 knowledge about pesticide behavior upstream APs. Nevertheless, little consideration has been
84 devoted to studying pesticides at the pond scale. Existing models such as AGRO-2014 and
85 TOXSWA are computationally costly because they require a significant number of inputs and
86 parameters and depend on other models' outputs (i.e., PRZM). In addition, AGRO-2014 only
87 accounts for hydrophobic pesticides. The lake-pond module of the Soil and Water Assessment
88 Tool (SWAT) can also simulate the fate of pesticides in APs. However, SWAT does not
89 integrate the effect of temperature and desorption and does not consider the kinetic effect of
90 adsorption-desorption, given that these factors are widely reported as key drivers of pesticides
91 fate (Burrows et al., 2002; Cryder et al., 2021; Kadlec and Wallace, 2008; Kaur and Kaur, 2018;
92 Papaevangelou et al., 2017; Vymazal and Brezinova, 2015).

93 On this basis, a descriptive model of pesticide fate in APs "*PESTIPOND*" was developed.
94 *PESTIPOND* is built upon simple mathematical formulation with a limited number of inputs
95 and parameters. Contrarily to black-box models considering a single decay rate of pesticides,
96 *PESTIPOND* is a process-based model integrating the key processes behind pesticide fate in
97 APs. *PESTIPOND* simulates the fate of different pesticides (hydrophobic and hydrophilic)
98 intercepted through agricultural water and distributed in the surface water and sediment
99 compartments of the AP. The key processes considered by the model are adsorption-desorption,
100 biotransformation in water and sediments, photolysis, hydrolysis, and volatilization.
101 *PESTIPOND* is designed to be implemented in a landscape model in fine (e.g., SWAT model)
102 to predict the transfer of pesticides at the watershed scale.

103 The model program was coded using the R language. The input data consists of 10 parameters
104 and 6 forcing variables listed in Table A.1. The model was previously tested on a test-case
105 scenario and successfully simulated the mass in water and sediments of dissolved pesticides
106 contained in agricultural drainage water, using arbitrary parameter values and observed data.
107 The development, testing, and sensitivity analysis (SA) of *PESTIPOND* can be found in (Bahi
108 et al., 2023, submitted). A module of *PESTIPOND* is dedicated to the reactive transport of
109 adsorbed pesticides, but due to a lack of observed data, it still needs to be completely validated.

110 The main hypotheses of the model are summarized hereafter:

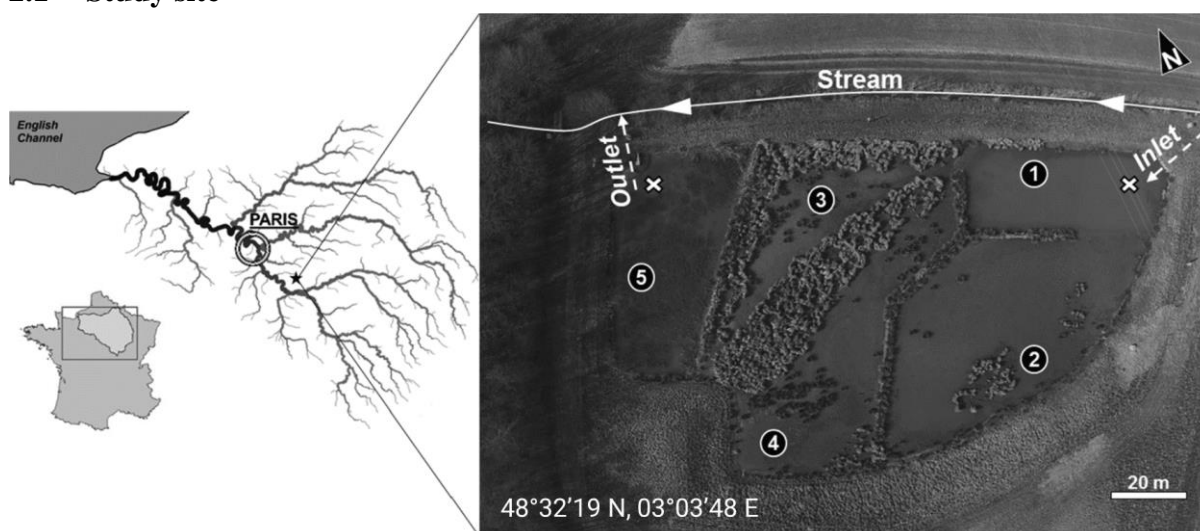
- 111 (1) Concentrations of pesticides are spatially uniform in water and sediments because the
112 AP compartments are considered completely mixed reactors. Hence, once pesticides
113 enter a specific compartment, they are instantly mixed with the entire content and
114 distributed uniformly. In practice, after several hours, the pond water becomes perfectly
115 mixed (Alvord and Kadlec, 1996; Pugliese et al., 2020). Besides, the pond
116 heterogeneities responsible for the non-uniformity of concentrations are usually
117 considered in hydraulics-based models (Henine et al., 2022) rather than chemical-based
118 models, e.g., for pesticides (Bahi et al., submitted, (Watanabe and Takagi, 2000b) and
119 nitrates (Hantush et al., 2013; Krone-Davis et al., 2013).
- 120 (2) Vegetation is not considered by the *PESTIPOND* model. Prior investigations have
121 evidenced that the fraction of pesticides collated in plants were often insignificant in
122 APs (< 10%) (Butkovskiy et al., 2021; Pérez et al., 2022; Singh et al., 2021; Wang and
123 Kelly, 2017). Not considering the vegetation implies neglecting its effect on the
124 hydraulic flow (brakes, dead zones). Nonetheless, this choice of hypothesis was
125 motivated by the environmental focus of the model rather than the hydraulic one, hence
126 also the hypothesis (1).

- 127 (3) No advection or diffusion processes are considered by the model for the following
128 reasons; (a) APs are often constructed on a compacted substrate where the infiltration
129 (leaching) is not significant, and the water velocity at the water-sediment interface is
130 too low resulting in a weak hydraulic gradient that limits advection in the sediment layer
131 and the water-sediment interface. In addition, the water velocity in the water column of
132 the evaluated APs is too low to induce advection of pesticides. (b) Several studies
133 showed that the molecular diffusion of diverse pesticides is too low in the water ($\sim 10^{-9}$
134 $\text{m}^2 \cdot \text{s}^{-1}$ at 25°C) (Chevillard et al., 2014; Fernández-Pascual et al., 2020; Sarraute et al.,
135 2019).
- 136 (4) PESTIPOND simulates the fate of pesticides in the first cm of sediments designated as
137 the active sediment layer governing pesticide transformation and transport under
138 flooded conditions. Previous in-situ measurements proffered that pesticide residues are
139 not significant beyond 1cm of depth (Inao and Kitamura, 1999; Mahugija et al., 2018;
140 Nyantakyi et al., 2022; Takagi et al., 2012). The pore water of the active sediment layer
141 is included in the water column compartment.
- 142 (5) Transformation and volatilization processes are corrected according to the temperature
143 change during the simulation period.
- 144 (6) Since the fate of metabolites is still poorly documented, PESTIPOND does not consider
145 transformation products.

146 The present paper addresses the application and validation of the PESTIPOND model regarding
147 the prediction of pesticide fate in APs. The model application and validation were performed
148 based on inputs from monitoring data in the Rampillon AP and parameter values calibrated or
149 extracted from literature. The model was validated upon 19 scenarios, where each scenario
150 corresponds to a specific pesticide and its corresponding monitoring period (Table A.8).

151 2 Materials and methods

152 2.1 Study site



153
154 **Figure 1:** Map visualizing the localization of the AP of Rampillon (Seine-et-Marne, France) within the Seine
155 River basin. Circled numbers indicate the different cells separated by bunds and considered for the spatial sampling
156 (Lebrun et al., 2019). The white arrows refer to the ditch from where the AP intercepts agricultural water.

157 The experimental set-up is at the Rampillon AP (5270 m^2), located in a 355-ha watershed
158 upstream of the *Ancoeur* agricultural catchment (132.2 km^2), 70 km southeast of Paris, France

159 (03°03' 37.300E, 48°32'16.700 N) (Fig.1). The AP occupies a 0.15% area of the alimentation
160 watershed and is situated on the Brie plateau subjected to intensive agriculture. The Rampillon
161 AP was implemented in 2010 to address local environmental and health issues (Lebrun et al.,
162 2019; Tournebize et al., 2017; Tournebize et al., 2012). It was designed to collect runoff and
163 drainage water sourcing from agricultural plots before being fed into the Champigny water
164 table, which constitutes a major drinking water resource. Almost 60% of the Champigny water
165 originates from direct infiltration of agricultural runoff through sinkholes (Fig.A.1). The
166 Champigny water table provides drinking water for almost 1.5 million citizens, hence the
167 priority to safeguard its quality by reducing pesticide transfer.

168 A typical waterlogging French soil characterizes the *Ancoeur* catchment. Therefore, more than
169 80% of the catchment and the whole Rampillon area have been subsurface drained since 1980
170 to prevent frequent winter soil saturation (Tournebize et al., 2012). The drains are perforated
171 pipes buried to a depth of 90 m and spaced 10 m apart. The 355-ha watershed receives an annual
172 mean rainfall of 689mm, and the annual mean drained flow is 228 mm. Farmers mainly grow
173 winter wheat, sugar beet, corn, beans, and rape. The Rampillon AP comprises sub-basins
174 separated by bunds to enhance pesticide dissipation and accumulation by increasing the water
175 residence time (HRT) (Tournebize et al., 2012). The first sedimentation basin is 100 cm deep
176 and 300 m³ (Fig.1; i.e., cell 1). The 4000-m² intermediate zone is a shallow sub-basin of a
177 maximum of 50cm deep, including cells 2, 3, and 4 (i.e., 1680, 1450, and 870m², respectively).
178 About 20, 60, and 50% of the inlet and outlet of cells 2, 3, and 4, respectively, were covered by
179 vegetation in 2015: reed (*Phragmites australis*), bulrush (*Juncus* spp.), and sedge (*Carex* spp.).
180 A final 1000-m³ basin, 80 cm deep (i.e., cell 5), was implemented before the outlet. The total
181 volume of the Rampillon pond is 2500 m³. Sediments of the AP are composed of coarse silt for
182 32.8%, clay for 27.8%, fine sand for 7.7% (3.5%), coarse sand for 2.7% (2%) through a transect
183 from inlet and outlet, and 2-2.8% for organic matter. The loamy texture of sediment is similar
184 to the surrounding soil texture. In 10 years, 10 cm of sediments accumulated in the Rampillon
185 AP. On average, the AP intercepts 40% of the collected drainage water with 30 000 m³ transited
186 per year.

187 2.2 Monitoring data

188 The Rampillon AP was initially implemented to buffer nitrate, metals, and pesticides
189 originating from intercepted agricultural water. Therefore, since 2012, the Rampillon AP is
190 instrumented to continuously monitor nutrient and pesticide fluxes and major water
191 physicochemical parameters (i.e., flowrate, temperature, and dominant ions) at the inlet and
192 outlet of the site (Fig.1). The typical monitoring stations comprise a flowmeter based at the
193 water level, a Doppler (Sigma 950, Hach), a multi-parameter spectrophotometer (Spectrolyser
194 UV-vis, S::can) for hourly measurements of turbidity and nitrates, and an automatic sampler
195 managed for bi-monthly flow-weight sampling strategies. IRIS (IRIS Instruments, Orleans,
196 France) also measured water temperature and water level using a pressure transducer model
197 Madofil close to the outlet. Rainfall data were obtained through a local pluviometer installed at
198 the study site. The daily potential evapotranspiration (PET) data are available in the
199 MétéoFrance SAFRAN database (Vidal et al., 2010). PET data values are calculated following
200 the Penman-Monteith formula. The hydrology of the 355-ha watershed is summarized in
201 Fig.A.2. It was chosen to validate the model upon the following five periods: 2014-2015, 2016-
202 2017, 2017-2018, 2018-2019, and 2019-2020 excluding monitoring periods with artifacts and
203 pesticide re-mobilization that is detailed afterward. The selection of the pesticide molecules for

204 the model validation is motivated by the diversity of their chemical properties and their
205 significant detection rate. The monitoring data of the 5270 m² AP during the selected periods
206 are summarized in Table A.8.

207

208 2.3 Input data

209 Since 2011, outlet and inlet pesticide concentrations have been monitored in the Rampillon AP.
210 The AP efficiency to mitigate pesticides is calculated from the mass fluxes using Eq.1. Note
211 that the mass flux corresponds to the total mass of pesticide detected in the water with no
212 distinction between the dissolved and particulate fraction.

213 (1)

$$214 \quad \text{efficiency (\%)} = \left(1 - \frac{\text{outlet mass flux}}{\text{inlet mass flux}} \right) * 100$$

215 Where the outlet and inlet mass fluxes (μg) are deduced from the concentrations ($\mu\text{g.L}^{-1}$).

216 Since the rate of pesticide mitigation varies with the type of pesticide, it is suitable to represent
217 the AP performance by a mean efficiency. Fig.A.3 depicts the total efficiency of the Rampillon
218 AP in dissipating each of the seven evaluated in this work. The main physicochemical
219 properties of the evaluated pesticides are listed in Table 1.

220 The monitoring data showed that, on average, the Rampillon AP dissipates 23% of the total
221 intercepted flux of selected pesticides. The highest dissipation rate (48%) goes to boscalid
222 during 2016-2017, followed by quinmerac (34%) and mesotrione (36%) during 2018-2019.
223 Mesotrione was dissipated by 33% equally during its two years of monitoring, i.e., 2017-2018
224 and 2018-2019. The mitigation of s-metolachlor varied sharply throughout the years, with a
225 dissipation rate going from 30% during 2016-2017 to 5% during 2014-2015 and 2019-2020. A
226 similar variation was noticed for quinmerac that was dissipated up to 36% during 2018-2019,
227 while its inlet mass was barely reduced during 2014-2015.

228 Compared to other periods, a significant efficiency was observed during 2016-2017 for
229 bentazon, boscalid, and s-metolachlor. The higher dissipation could result from the high HRT
230 (14 days), and temperature noticed back then (11°C). Similarly, mesotrione and quinmerac were
231 significantly dissipated during 2018-2019, which had an average HRT of 9 days. In fact, a
232 longer HRT provides time for accumulation and transformation processes behind pesticide
233 dissipation, and a higher temperature stimulates the microbial activity behind pesticide
234 biotransformation and is associated with significant solar radiation responsible for
235 photodegradation. This observation ties in with other studies demonstrating that temperature
236 and HRT are major drivers of pesticide behavior in AP (Bahi et al., 2023b; Imfeld et al., 2021;
237 Materu et al., 2021; Pavlidis et al., 2022; Vallée, 2015). Interestingly, mesotrione had a mean
238 dissipation of 50% during a lower mean temperature (9°C) and HRT (7 days). It could be
239 explained by the high biodegradability of the molecule evidenced by short half-lives in both
240 sediment and water, 5.3 and 5.2, respectively (Lewis et al., 2016). These observations underline
241 the potential relationship between pesticide properties, hydro-climatic conditions, and APs
242 performance. Therefore, this relationship will be evaluated using the PESTIPOND model
243 (section 4).

244

245 **Table 1:** The physicochemical properties and the application season of the 7 studied pesticides. K_{oc} (mg.L^{-1}) is the
 246 organic carbon-water partition coefficient, representing the mobility of the molecule. $\log Kow$ (-) is the octanol-
 247 water partition coefficient, representing the hydrophobicity of the molecule. S (mg.L^{-1}) is the water solubility of
 248 the molecule, and LOD ($\mu\text{g.L}^{-1}$) is the detection limit of the molecule in water. The properties values were extracted
 249 from literature (Barchanska et al., 2012; Catalá-Icardo et al., 2015; Epa, 2001; Lewis et al., 2016; PubChem, 2021)
 250 and the application season was deduced from a follow-up of cultural practices in Rampillon.

Pesticides	K_{oc}	$\log Kow$	S	LOD ($\mu\text{g.L}^{-1}$)
Bentazon	55	2.34	7112	0.005
Boscalid	772	2.96	4.6	0.016
Chlorotoluron	400	2.41	76	0.03
Diflufenican	550	4.2	0.05	0.07
Mesotrione	122	0.11	1500	0.04-0.61
S-Metolachlor	120	2.9	480	0.02
Quinmerac	86	2.7	107000	0.0006

251

252 In terms of the detection frequency of each pesticide, bentazon was the most frequently detected
 253 pesticide, which may be due to its wide range of application periods, i.e., March, April, May,
 254 and June. Similarly, diflufenican was highly detected in the Rampillon AP because it was
 255 applied during three seasons, i.e., autumn (October and November), winter (January and
 256 February), and spring (March). A similar explanation can be accorded to quinmerac applied
 257 during autumn (September and October), spring (March, April, and May), and summer (June).
 258 On the other hand, Boscalid was only detected during 2014-2015 and 2016-2017. In fact,
 259 boscalid was always applied in April and once in May; therefore, if the application did not co-
 260 occur with an important spring rainfall event, the pesticide in question would be unlikely to be
 261 detected in drainage water. Moreover, due to its K_{oc} (772 L.kg^{-1}) boscalid has a higher affinity
 262 to sediments, reducing its availability in the water reaching the pond. Likewise, mesotrione
 263 although being applied more frequently, it was only detected twice (2017-2018, 2018-2019).
 264 Mesotrione was applied during spring and summer (March, April, and June), with a low
 265 incidence of flooding events explaining the molecule's infrequent detection.

266 The AP efficiencies were calculated based solely on the pond inlet and outlet amount of
 267 pesticides. It is; therefore, unknown which processes are driving the dissipation of pesticides.
 268 Therefore, the purpose of the PESTIPOND model is to simulate the behavior of pesticides and
 269 quantify the contribution of each process to the pesticide fate in APs. Hereafter are detailed the
 270 model inputs, i.e., forcing variables and parameters.

271 2.3.1 Forcing variables

272 The list of the forcing functions required by the model is provided in Table A.1. It is important
 273 to recall that inlet and outlet concentrations are observed bi-monthly at the study site. The
 274 concentrations collected each fortnight are the average intercepted concentrations during the
 275 past two weeks. Therefore, to have a close insight into pesticide behavior and the model
 276 simulations, the bi-monthly observed concentrations were transformed to daily concentrations
 277 using a water flow rate weighted interpolation. The transformation method is detailed in (Bahi
 278 et al., 2023a). The daily inflow and outflow rates (Q_{in} , Q_{out}) were calculated from the hourly
 279 water flow rates measured on-site. The water flow rates are used to compute the inlet and outlet
 280 daily mass fluxes from the corresponding concentrations.

281 M_{in} ($\mu\text{g.d}^{-1}$) and M_{out} ($\mu\text{g.d}^{-1}$) are the daily mass fluxes of the pesticide at the AP's inlet and
 282 outlet. C_{in} ($\mu\text{g.l}^{-1}$) and C_{out} ($\mu\text{g.l}^{-1}$) are the daily concentrations at the inlet and outlet of the AP,

283 respectively. The water volume V_w was computed by the hydrological model detailed in (Bahi
284 et al., 2023a). The hydrological model of PESTIPOND requires daily local rainfall and
285 evaporation data, which were provided by SAFRAN (Vidal et al., 2010), along with the daily
286 temperature T ($^{\circ}\text{C}$), which corresponds to a measurement station nearby the Rampillon AP. The
287 water depth h_w (m) was deduced by Eq.2.

288 (2)

$$289 \quad h_w(t) = \frac{V_w(t)}{A}$$

290

291 V_w (m^3) is the water volume in the AP, and A (m^2) is the measured surface area of the AP.

292 2.3.2 Parameters

293 For the model validation, parameters were either extracted from the pesticide properties
294 database (PPDB) (Lewis et al., 2016) or calibrated, and the AP properties were measured on-
295 site (i.e., (Surface $A=5270 \text{ m}^2$ and the bulk density $\rho_b=0.9 \text{ g.cm}^{-3}$). The temperature correction
296 coefficient θ (see equation in (Bahi et al., 2023a)) is extracted from the literature (Sharifi et al.,
297 2013). The list of the model input parameters is available in Table A.1.

298 The parameters related to the processes were extracted from the PPDB and calibrated if not
299 available or if calibration would ameliorate the model performance. The calibration was
300 performed manually and numerically using the hydroGOF R-package (Zambrano-Bigiarini,
301 2020). The R-calibration function seeks the set of parameters leading to the best possible
302 performance of the model according to an evaluation criterion (e.g., NSE and KGE (Eq.3 and
303 Eq.4)).

304 The model parameters are classified in terms of processes: adsorption-desorption (k_{ads} (d^{-1}) and
305 k_{des} (d^{-1}) for sediment layer) and transformation processes ($\text{DT}_{50,w}$, $\text{DT}_{50,s}$ and $\text{DT}_{50,p}$. A
306 pesticide half-life (DT_{50}) is the time required for the dissipation of 50% of the substance concerned
307 (Gregoire et al., 2009) in water ($\text{DT}_{50,w}$), sediments ($\text{DT}_{50,s}$), and due to photolysis ($\text{DT}_{50,p}$).

308 The sensitivity analysis results (Bahi et al., 2023, *submitted*) evidenced that the PESTIPOND
309 model is insensitive to volatilization and hydrolysis independently of the pesticide molecular
310 properties. Therefore, based on literature values (Jacobs and Adriaanse, 2012; Rose et al.,
311 2006), volatilization and hydrolysis rate coefficients were given a fixed value for the rest of the
312 study ($k_v = k_h = 10^{-6} \text{ d}^{-1}$), leaving only 5 parameter values to determine ($\text{DT}_{50,w}$, $\text{DT}_{50,s}$, $\text{DT}_{50,p}$,
313 k_{ads} , and k_{des}). The parameter values used to assess the PESTIPOND model are to be found in
314 the result section (section 3).

315

316 2.4 Model validation strategy

317 The validation of the PESTIPOND model is based on the assessment of the simulations of
318 pesticide fluxes against the available observations using the 20 study cases (Table A.8). Other
319 pesticide fate models (Kalin et al., 2013; Watanabe and Takagi, 2000a) were validated using a
320 single pesticide molecule or a single period to evaluate the model performance. Alternatively,
321 PESTIPOND was validated upon field monitoring data of 7 pesticides with contrasting
322 molecular properties (i.e., solubility, hydrophilicity, and mobility) (Table 1) during the 5

323 evaluated periods. The split-simple test (SST¹) (Klemeš, 1986) is a common evaluation method
324 for this type of model. However, the SST requires sizeable observation data. Even though the
325 monitoring database of the Rampillon AP is consistent (2011-2022), it includes periods of no
326 application nor flooding events responsible for pesticide transfer, which restrains the database
327 size for SST use.

328 The validation strategy of the PESTIPOND comprises two steps (i) and (ii):

329 (i) Based on the observations of pesticide concentrations, the model parameters are
330 optimized for each period (i.e., annual parameters) to assess their stability and
331 consistency. The variability of parameters between periods indicates the degree of the
332 model's robustness.

333 (ii) In order to survey the parameters' variability and assess the model robustness, the
334 performance of PESTIPOND is evaluated using a single set of parameters (inter-annual)
335 for all periods (i.e., the mean value of the annual parameters).

336 Note that for (i) and (ii), the model performance is assessed using both the transformed
337 observations (daily observations) and the non-transformed observations (bi-monthly
338 observations). When the model is validated for the bi-monthly observations, a bi-monthly flow-
339 weighted concentration is calculated from the daily simulation results to match the
340 observations' time scale.

341 To quantitatively assess model performance, the well-known Nash Sutcliffe efficiency (NSE)
342 objective criterion (Nash and Sutcliffe, 1970) (Eq.3) was adopted. An additional metric was
343 used to assist the NSE criterion, i.e., Kling–Gupta efficiency (KGE) criteria (Gupta et al., 2009)
344 (Eq.4). The two criteria are known for properly evaluating nutrients and chemical fate models
345 (Moriasi et al., 2015). The NSE and KGE values range from $-\infty$ to 1 and require data on both
346 simulated and observed pesticide fluxes. NSE and KGE values close to 1 imply that the model
347 simulations fit the observations owing to good model performance.

348 The renowned *t*-test (the Student's statistical test) was used to evaluate the similarity between
349 observed and simulated pesticide concentrations (Stokes et al., 2014). Then, a regression
350 analysis was conducted to assess the correlation between the observed and simulated pesticide
351 concentrations (Montgomery et al., 2021). The *t*-test is a hypothesis-based test to compare the
352 means of two groups (e.g., observations and simulations). The test statistics are quantified by
353 the *t*-value (Eq.5) and *p*-value. A low *t*-value indicates a slight difference between the means
354 of both observations and simulations. A *p*-value higher than the significance level ($\alpha=0.05$)
355 means the null hypothesis cannot be rejected (Mishra et al., 2019). The test's null hypothesis is
356 that there is no significant difference between the two groups (Pieri et al., 2007; Serrano, 2012;
357 Wright et al., 2017). To further assess the relationship between observations and simulations, a
358 regression analysis was conducted and quantified by the R^2 (Eq. 6), where *R* is the Bravais-
359 Pearson correlation coefficient (Pearson, 1895; Waldmann, 2019). The higher the R^2 , the more
360 pronounced the correlation between the observed and simulated pesticide concentration. This
361 correlation is statistically significant when the *p*-value of the Pearson test is lower than 0.05.
362 The normalized root means square error (NRMSE) (Eq.7) was also computed to describe the

¹ The split sample test consists in splitting the observation data into two periods. The parameters are calibrated over the first period. Next, the model performance is evaluated by running the calibrated set of parameters obtained over the second period.

363 discrepancy between the observations and simulations. Since molecules have different
 364 concentration ranges, it is statistically more appropriate to compare the NRMSE than the regular
 365 RMSE ($\mu\text{g}\cdot\text{L}^{-1}$). Therefore, NRMSE was calculated by normalizing the RMSE according to the
 366 difference between the maximum and minimum concentrations for each pesticide (Kenney and
 367 Keeping, 1962; Sinsomboonthong, 2022). The statistical tests were performed using the “stats”
 368 R-package (Lüdecke et al., 2021).

369 (3)

$$371 \quad NSE = 1 - \frac{\sum_{t=1}^{t=T} (X_t - X_t^*)^2}{\sum_{t=1}^{t=T} (X_t^* - \overline{X_t^*})^2}$$

370 (4)

$$373 \quad KGE = 1 - \sqrt{\left(\frac{cov(X_t^*, X_t)}{\sigma(X_t^*)^2 \sigma(X_t)^2} - 1\right)^2 + \left(\frac{\overline{X_t}}{\overline{X_t^*}} - 1\right)^2 + \left(\frac{\sigma(X_t)}{\sigma(X_t^*)} - 1\right)^2}$$

372 (5)

$$374 \quad t = \frac{\overline{X_t} - \overline{X_t^*}}{\sqrt{\frac{\sigma(X_t)}{n} + \frac{\sigma(X_t^*)}{n}}}$$

375 (6)

376

$$377 \quad R^2 = 1 - \frac{\sum (X_t - X_t^*)^2}{\sum (X_t - \overline{X_t})^2}$$

378 (7)

$$379 \quad RMSE = \sqrt{\frac{1}{T} \sum_{t=1}^T (X_t - X_t^*)^2}$$

$$380 \quad NRMSE = \frac{RMSE}{\max(X_t) - \min(X_t)}$$

381 Where, X_t^* and X_t correspond to the observations and the simulations at the time step t ,
 382 respectively. $\overline{X_t^*}$ and $\overline{X_t}$ are the mean values of the observed and simulated pesticide fluxes,
 383 respectively, throughout the whole period of interest T . $cov(X_t^*, X_t)$ refers to the covariance
 384 between X_t^* and X_t while σ indicates the standard deviation. n is the size of the
 385 observation/simulation sample.

386

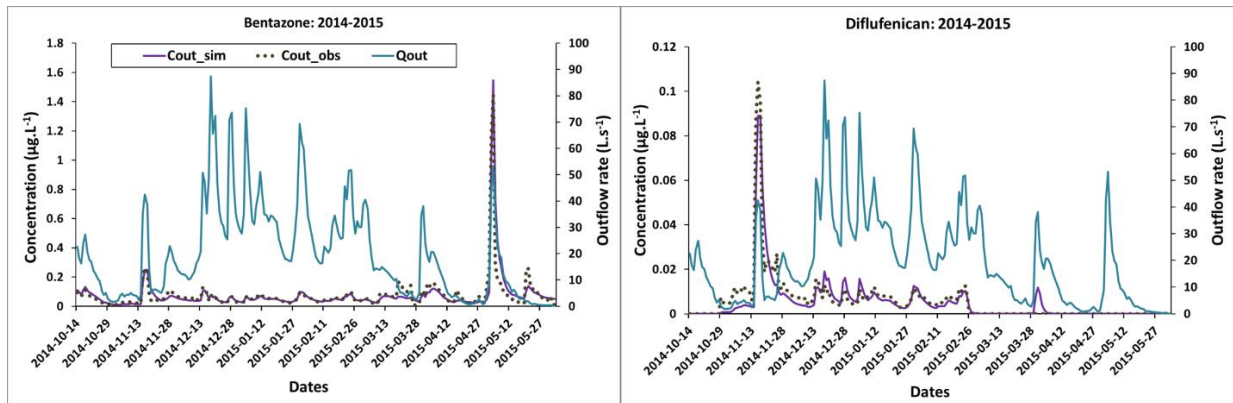
388 3 Results

389 3.1 Model assessment based on the annual calibration

390 An annual calibration of the model parameters according to pesticide fluxes is performed over
391 the selected periods. The obtained parameter values are set out in Tables A.2 & A.3.

392 A graphical and numerical comparison between simulations and observations of pesticide
393 fluxes at the AP outlet were carried out. First, the model performance was assessed according
394 to the daily observations, i.e., the transformed observations from the bi-monthly mean values
395 to daily values (Fig.2). Then according to the bi-monthly observations, i.e., non-transformed
396 observations, while using an annual calibration (Fig.A.5).

397 For brevity and representability, we only exhibit the results of two pesticides during 2014-2015,
398 i.e., the hydrophobic and slightly mobile diflufenican ($K_{oc} \text{ (L.kg}^{-1}\text{)} = 550$, $\log K_{ow} = 4.2$) and
399 the hydrophilic and highly mobile bentazon ($K_{oc} \text{ (L.kg}^{-1}\text{)} = 55$, $\log K_{ow}=2.34$) (Lewis et al.,
400 2016) (Fig.2).



401
402 **Figure 2** Graphical comparison of the daily simulations (purple line) and transformed observations (dark points)
403 of the bentazon and diflufenican concentrations in the outlet and the observed outflow rate (blue line).

404 From the graphical (Fig.2) and numerical outcomes (Table 3), it can be noted that the annual
405 calibration results in proper model performance. The KGE and NSE values are >0.5 , and the
406 RMSE does not exceed 0.07. Considering how wide the goodness-of-fit-range of variations are
407 (NSE $(-\infty, 1]$ and KGE $(-\infty, 1]$), the model performance can be considered as “good” due to the
408 annual calibration (Lee et al., 2021; Moriasi et al., 2007; Moriasi et al., 2015).

409
410 The simulations of the daily concentrations and masses of bentazon and diflufenican align with
411 the observations. The outlet concentrations increase after the pesticide application, i.e., during
412 spring for bentazon and autumn for diflufenican (Fig.2). The model simulates the higher
413 exportation of bentazon (40g) in the water compared to diflufenican (3.5g) during 2014-2015.
414 During the same year, quinmerac was also exported significantly, with a total mass of 43g,
415 while the exportation of the other pesticides (i.e., boscalid, chlorotoluron, and s-metolachlor)
416 did not exceed 10g (Fig.A.4).

417
418 However, the model underestimated almost equally the overall exportation of s-metolachlor
419 and quinmerac with a discrepancy of 3g, which covers 5% and 22% of the total intercepted
420 mass, respectively, during 2014-2015. For the rest of the periods and pesticides, the model

421 managed to reproduce the observed mass exportation. Fig.A.4 displays that the model simulated
422 the lower AP efficiency in dissipating the mass of mesotrione, s-metolachlor, and quinmerac
423 during 2017-2018. During the same year, PESTIPOND also simulates the highest exportation
424 for s-metolachlor (300g). Globally, the simulation results reflect a lower performance at higher
425 concentrations following pesticide applications compared to lower concentrations (Fig.2).

426
427 The results underline that the simulations with the annually calibrated set of parameters also fit
428 the non-transformed observations (bi-monthly) of pesticide concentrations (Fig.A.5). The
429 simulated concentration of s-metolachlor was underestimated compared to the observations of
430 two samplings (22/05/2017 and 19/05/2020). Similar underestimation was noted for s-
431 metolachlor mass exportation in Fig.A.4, which is also translated by its lower KGE (0.53)
432 compared to other pesticides (Table 3). Conversely, the model overestimated the concentration
433 of boscalid during 2014-2015 and 2016-2017. This overestimation also concerned the exported
434 boscalid mass during 22/02/2017-20/03/2017 and 22/02/2017 (Fig.A.4). Accordingly, boscalid
435 had the lowest KGE (0.44) (Table 3).

436
437 On average, an annual parameter calibration induces a discrepancy between simulated and
438 observed fluxes of 0.03g, all periods and pesticides included. Overall, the graphical comparison
439 evidences the ability of the model to predict the dynamics of the outlet concentrations (Fig.2),
440 and to simulate the concentrations observed in the field (Fig.A.5). The KGE and NSE criteria
441 reflect a good performance of the PESTIPOND model according to the annual calibration,
442 except for boscalid (Table 3).

443 **3.2 Model assessment based on the inter-annual calibration**

444 The adsorption-desorption parameter (k_{ads} , k_{des}) vary more pronouncedly over the years than
445 transformation ones ($DT_{50,w}$, $DT_{50,s}$, and $DT_{50,p}$) (Tables A.2 & A.3). In order to evaluate this
446 variability, we ran the model using a generic set of parameters (Table 3), which is the mean
447 value of the annual-calibrated parameters (Tables A.2 & A.3) and estimated the performance
448 criteria (Table 3). Additionally, a graphical comparison between the simulations using the
449 calibrated parameters and the non-transformed observations is provided (Fig.3).

450

451 **Table 2:** The mean value of the annual-calibrated parameters, and the PPDB values of transformation half-lives,
 452 i.e., (DT_{50,w}, DT_{50,s}, and DT_{50,p}). The physicochemical properties were extracted from the PPDB or other pesticide
 453 databases if not available.

Pesticides	Calibrated					PPDB			PPDB/Literature	
	DT _{50,w}	DT _{50,s}	DT _{50,p}	k _{ads}	k _{des}	DT _{50,w}	DT _{50,s}	DT _{50,p}	K _{oc}	log K _{ow}
Bentazon	5	100	3	0.15	0.01	80	716	4	55	2.34
Boscalid	500	500	stable	0.63	0	5	545	stable	772	3
Chlorotoluron	44	300	30	0.42	0	44	308	30	400	2.5
Diflufenican	200	175	133	0.51	0	200 ²	175	stable	550	4.2
Mesotrione	5.3	5.2	89	0.69	0.05	5.3	5.2	89	122	0.11
S-metolachlor	1.5	43	146	0.07	0.01	9	43	146	120	2.9
Quinmerac	3.84	180	66	0.43	0.02	88	179	66	86	2.7

454

455 **Table 3:** Statistical comparison of simulations and daily observations of pesticide fluxes. The left part of the
 456 table lists the KGE, NSE, and NRMSE values using an inter-annual set of parameters, i.e., the mean of the
 457 annual-calibrated parameter values, and the right part is for the annual calibration

Pesticides	Inter-annual calibration			Annual calibration		
	KGE	NSE	NRMSE	KGE	NSE	NRMSE
Bentazon	0.74	0.79	0.07	0.75	0.79	0.07
Boscalid	0.44	0.64	0.06	0.68	0.68	0.06
Chlorotoluron	0.74	0.87	0.01	0.83	0.82	0.05
Diflufenican	0.76	0.78	0.07	0.74	0.73	0.05
Mesotrione	0.63	0.93	0.03	0.69	0.87	0.04
S-metolachlor	0.58	0.76	0.04	0.58	0.75	0.05
Quinmerac	0.54	0.84	0.04	0.65	0.86	0.04

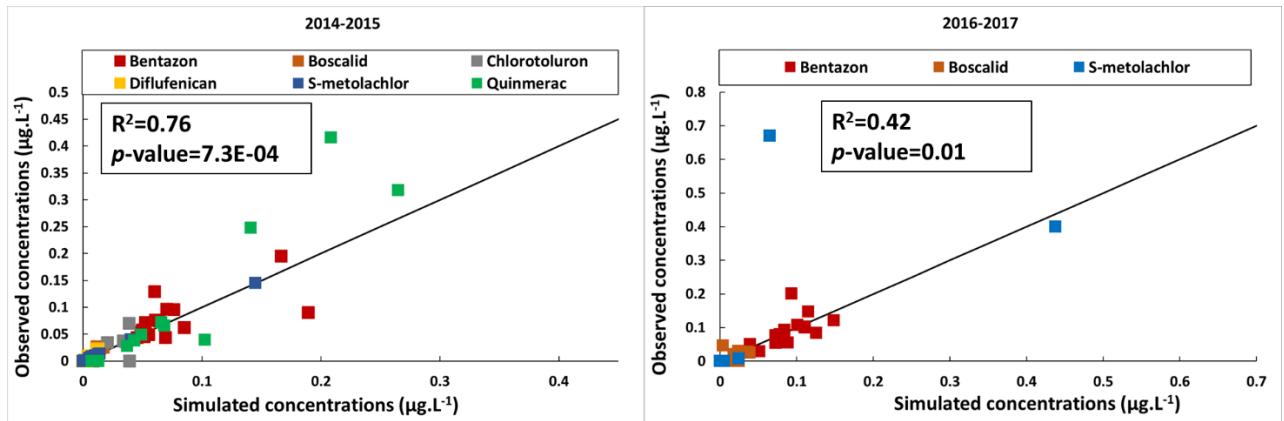
458

459 High KGE (>0.5) and NSE (>0.6) values of the model outputs were observed when using the
 460 inter-annual set of parameters for all pesticides (Table 3). Boscalid made the exception with a
 461 KGE of 0.44. Given that the annual calibration was designed to find a proper set of parameters
 462 for each period (Tables A.2 & A.3), the performance was expected to decrease when running
 463 the model with a single set of parameters independently of the period (Table 2). Nonetheless,
 464 the criterion values reflect in aggregate a good model performance, i.e., NSE >0.35 and KGE
 465 >0.5, except for boscalid, which indicates a not satisfactory performance according to the
 466 commonly used thresholds (Knoben et al., 2019; Moriasi et al., 2015; Towner et al., 2019).

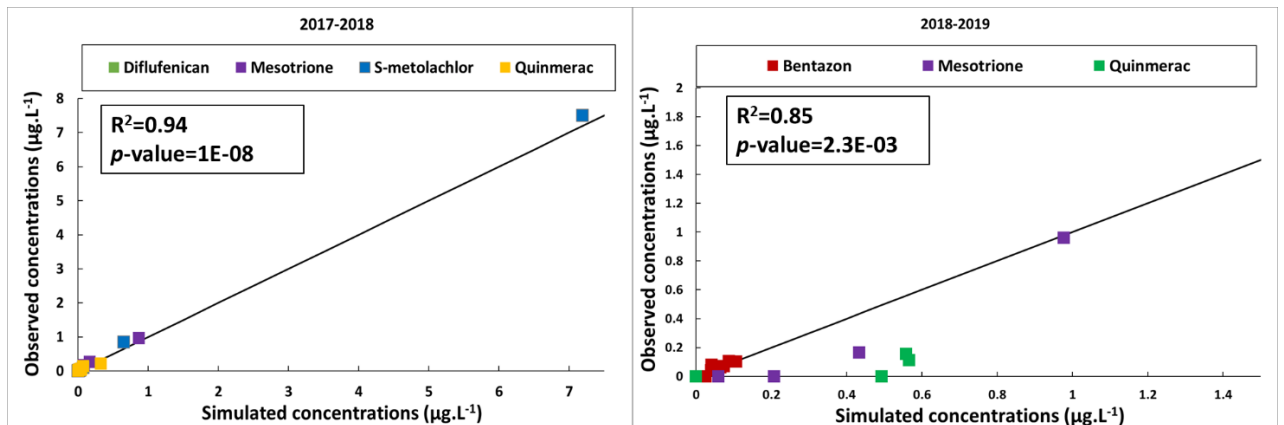
467

² The biotransformation half-life in water of diflufenican was not available in the PPDB so it was extracted from EFSA (2008). Conclusion regarding the peer review of the pesticide risk assessment of the active substance diflufenican. *EFSA Journal* 6, 122r.

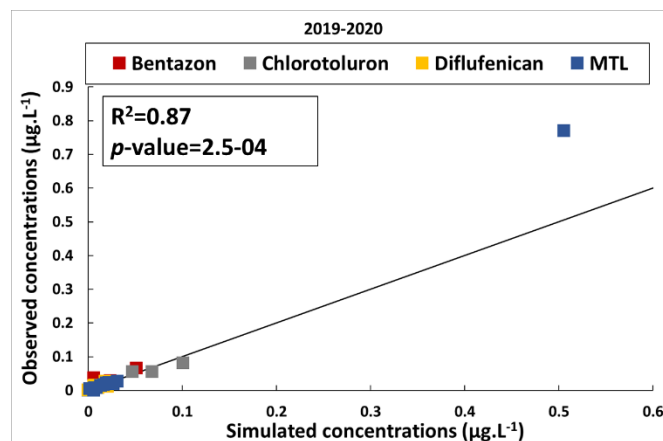
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469



470



471 **Figure 3:** Graphical comparison of the bi-monthly observations (y-axis) and simulations (x-axis) of all pesticide
 472 outlet concentrations ($\mu\text{g.L}^{-1}$) and periods combined, using the inter-annual calibration. Each color points out a
 473 specific pesticide. The black line in the middle refers to simulations equal to observations ($Y=X$). R^2 is the R-
 474 squared correlation coefficient between the observations and simulations. p -value³ is the p -value of the regression
 475 test.

476 Using the inter-annual set of parameters results in a good fit between the simulations and the
 477 non-transformed observations of pesticide concentrations (Fig.3). The R^2 values were >0.7 (p -
 478 values <0.05), indicating a strong correlation between the observations and simulations, except
 479 during 2016-2017 ($R^2=0.41$). The s-metolachlor simulated concentration ($0.5\mu\text{g.L}^{-1}$) was
 480 underestimated compared to the observations ($0.77\mu\text{g.L}^{-1}$) during 2019-2020. The
 481 underestimation was more accentuated during 2016-2017 when the simulated concentration of
 482 s-metolachlor ($0.06\mu\text{g.L}^{-1}$) was ten times lower than the observations ($0.67\mu\text{g.L}^{-1}$). The poor

³ A p -value <0.05 indicates that the correlation between the observations and simulations is statistically significant.

483 performance of the model evidenced by the low KGE value of boscalid is also noticed by the
484 overestimation of the exported mass during 2016-2017 and the pronounced underestimation
485 during 2014-2015 (Fig.A.6). On average, the relative error of boscalid discharge simulations is
486 36% while it is <10% for other pesticides. The *p*-values of the *t*-test were >0.05, reflecting that
487 the null hypothesis cannot be rejected (Table A.4). Hence, there is no significant difference
488 between the observed and simulated pesticide concentration for all periods. The high R^2 values
489 indicate a strong correlation between the observed and simulated pesticide concentration,
490 except for 2016-2017, manifesting a moderate correlation—the *p*-values of the regression
491 analysis evidence the statistical significance of these correlations (Table A.4).

492 Altogether, the graphical and statistical comparison of the observations and the simulations
493 using the inter-annual set of parameters reflect a good model performance for all pesticides
494 except for boscalid. After the quantitative evaluation of the model, the next section will describe
495 the mass budget of pesticides within the AP and the contribution of each process to pesticide
496 dissipation.

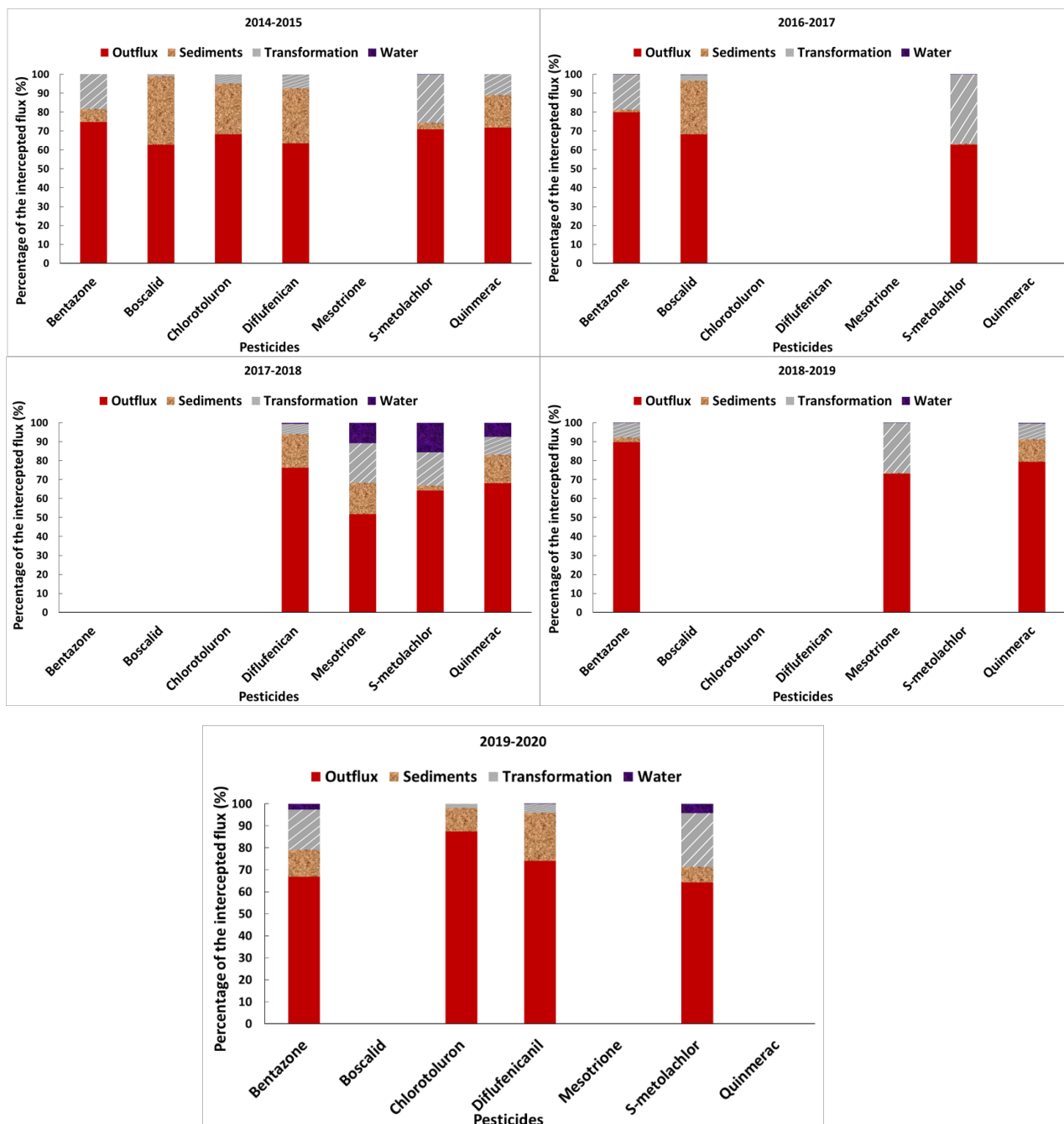
497 **3.3 Pesticide mass budget**

498 One of the PESTIPOND model's major aims is to quantify each process's contribution to the
499 fate of pesticides. Accordingly, after running the model with the mean set of parameters, the
500 mass budget of pesticides was assessed to illustrate the mass distribution in the pond and the
501 contribution of each process to pesticide dissipation. Table A.5 summarizes the mass budget
502 for all the pesticides and periods of the survey. Note that the PESTIPOND model checks
503 whether the mass balances tally during the calculations. The mean mass balance error of the set
504 of pesticides and periods is <1 % showing that the model conserves the mass properly.

505 For succinctness, only mean values of the mass partition in the AP at the end of each period
506 will be discussed in the following (Fig.4). Note that the transformation in water includes the
507 biotransformation, photolysis, hydrolysis, and volatilization in the water column.

508 Overall, most intercepted pesticides are discharged from the pond with a mean out flux of 72%,
509 followed by the mass remaining in the active sediment layer with a mean proportion of 12%,
510 which leaves almost 2% pesticides in the water column. Therefore, the mean dissipated mass
511 between the inlet and outlet of the AP accounts for 14% of the total intercepted mass.

512



513

514

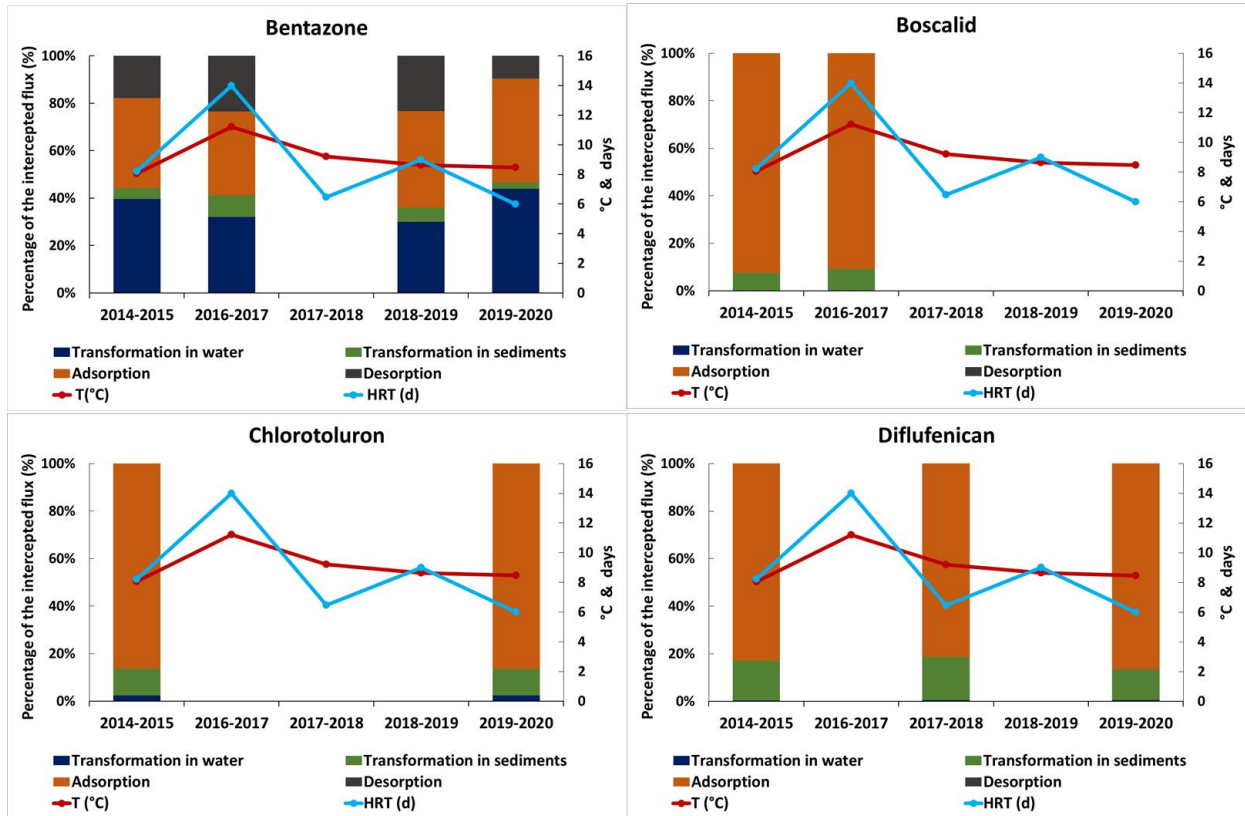
515

516 **Figure 4:** Graphical representation of the proportion of pesticide masses to the total input mass.

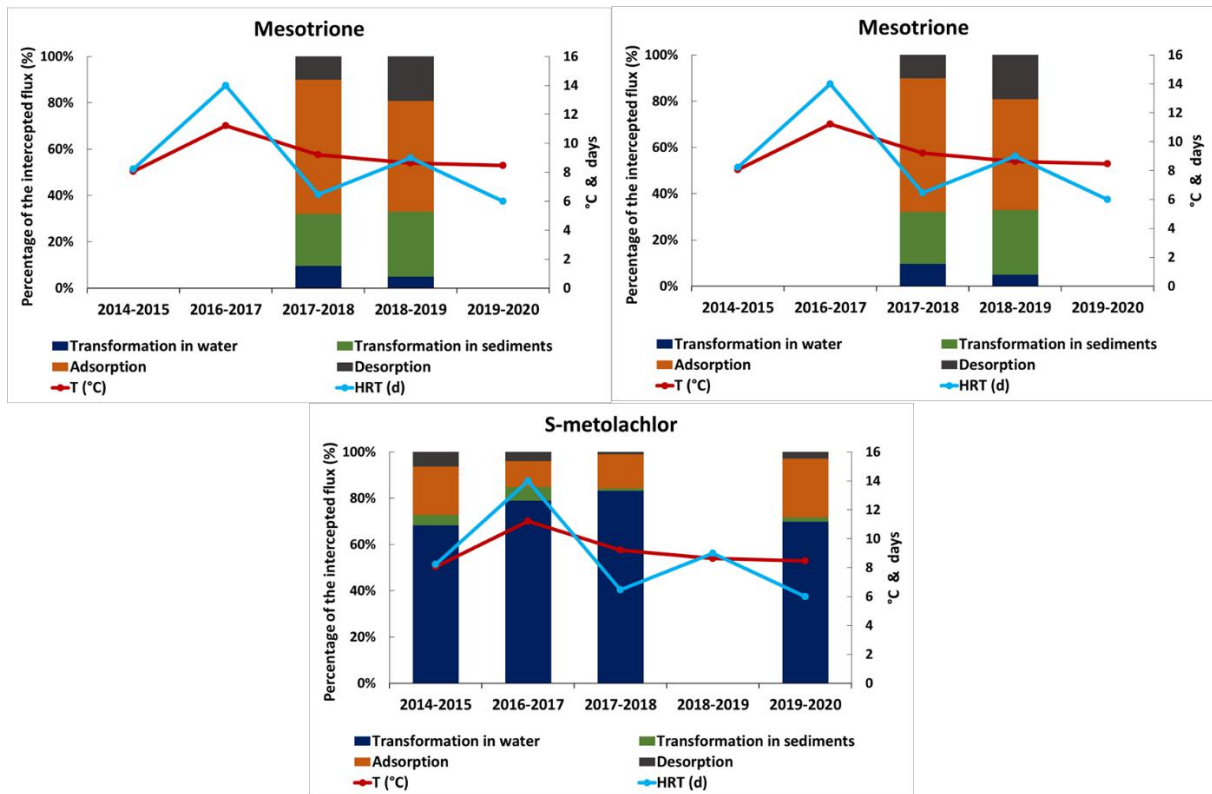
517 On average, boscalid, mesotrione, and quinmerac had the highest adsorption (Fig.4), which
 518 covers 35%, 36%, and 35% of the total input mass, respectively (Table A.5). Diflufenican,
 519 chlorotoluron, and bentazon come after with adsorption of 28%, 21%, and 14%, respectively.
 520 S-metolachlor had the lower adsorption (6%) but a significant transformation in water (24%),
 521 which is mostly due to biotransformation (23%), leaving only 1% to the other transformation
 522 processes (photolysis, hydrolysis, and volatilization). A significant transformation in the water
 523 column was also noted for bentazon (14%), which is mainly partitioned between photolysis
 524 (9%) and biotransformation (5%). On the other hand, biotransformation at the water-sediment
 525 interface had an important contribution to pesticide dissipation. For instance, 18% of the
 526 mesotrione intercepted mass was biodegraded on average in the active sediment layer.

527 Moreover, during 2014-2015, boscalid, chlorotoluron, and diflufenican were more transformed
 528 in the sediments than in water. The transformation in water and desorption rates for the same
 529 three pesticides are negligible (<1%). Conversely, the quinmerac desorption covers 20% of the
 530 inlet mass, followed by mesotrione (10%) and bentazon (7%). The photolysis contribution to
 531 dissipation was negligible for all pesticides except for the bentazon (8%).

532 Temperature was the highest during 2016-2017, which overlapped with the highest, desorption
 533 and transformation of bentazon at the water-sediment interface. The same period exhibited the
 534 highest HRT.



535



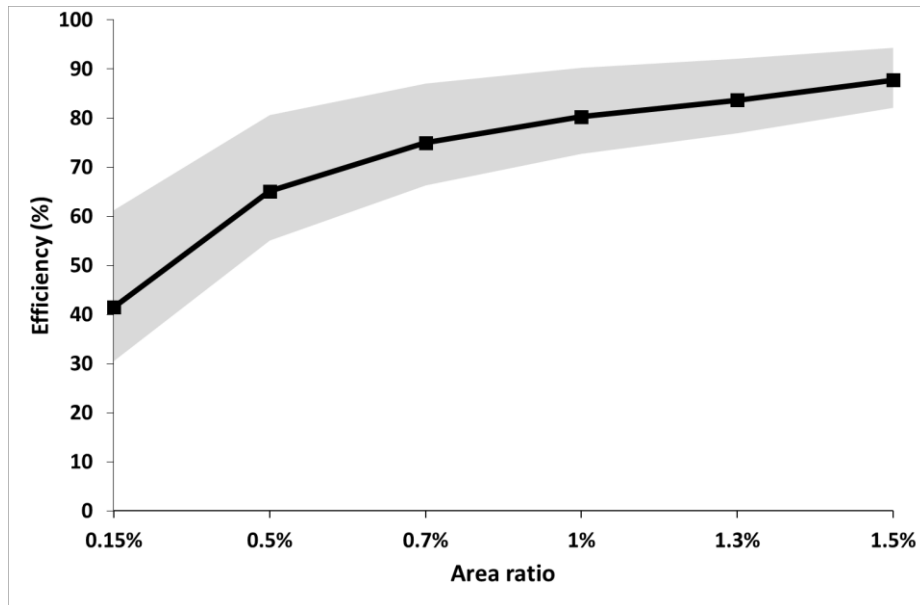
536

537 **Figure 5:** Graphical representation of the percentage of each process to the total mass intercepted by the pond and,
 538 the average temperature T (°C) and HRT (d) of each period.

539 3.4 Model extrapolation: Efficiency abacus

540 For further exploitation of the model outputs, PESTIPOND was run with the inter-annual
 541 parameter set described in section 3.3 and the same inputs presented in Section 2.3 but using
 542 different AP sizes in ascending order, equivalent to higher nominal HRT. For each simulation
 543 assigned to a specific AP area A (and HRT), the mean pesticide dissipation efficiency was
 544 computed (Eq.1). For the different simulations, only the AP area was modified, and the rest of
 545 input data were kept the same (e.g., the water flow rates, water depth, and temperature).

546 Note that a mean efficiency, including all pesticides, is computed for each period, and then a
 547 mean value for all periods is deduced (Fig.6, Table. A.7).. For this extrapolation study, ,
 548 boscalid was excluded because it yielded poor model performance (section 3.2).



549

550 **Figure 6:** The mean efficiency of the Rampillon AP to dissipate pesticides from the inlet to the outlet according to the different sizes of the pond. The x-axis represents the percentage (%) of the area occupied by the AP in the
 551 total catchment area (355ha). The y-axis corresponds to the mean efficiency of the studied periods. The upper and
 552 lower grey areas refer to the discrepancy between the mean and the maximum and minimum efficiencies,
 553 respectively.
 554

555 For the actual Rampillon area (5270m²), which covers 0.15% of the drained catchment area
 556 (355ha), the mean AP efficiency is 40% for all pesticides combined. By increasing the surface
 557 area by 10 000 m², the HRT is tripled, and the efficiency rises sharply to 63%. From an area
 558 that covers 0.7% of the watershed, the efficiency increases less steeply and attains about 82%
 559 (Fig.6).

560 An annual variation of the simulated pond efficiency independently of the area was noticed
 561 (Fig.A.8). However, the variation degree decreased with increasing pond areas, as well as the
 562 efficiency itself, as observed in Fig.6. For the actual AP size (i.e., 0.15% of the catchment area),
 563 the efficiency doubled from 2014-2015 (30%) to 2016-2017 (62%). Afterward, the dissipation
 564 potential of the pond decreased sharply to 36% during 2017-2018 and remained around 38%
 565 for the following years. Similar behavior will be noticed in the pond's efficiency if the surface
 566 increases to 0.5%-0.7% of the catchment area, with higher minimum and (55%-66%) and
 567 maximum values (80%-87%), respectively. For a ratio of 0.15%-0.7%, the mean pond
 568 dissipation is 17% lower than the mean maximum and 10% higher than the minimum.
 569 Conversely, once the AP area covers >1% of the catchment, the discrepancy between the mean
 570 efficiencies and the minimum and maximum values decreases to ~8% and ~6%, respectively
 571 (Fig.6).

572 In addition, similar extrapolation was performed on different temperatures representing a
 573 geographical temperature gradient (Fig.A.9). Pesticide dissipation increases linearly according
 574 to ascending temperature. On average, the current temperature of the surveyed periods is 9°C,
 575 which results in a 40% efficiency of the Rampillon AP.. In aggregate, a temperature rise of 5°C
 576 will boost the mean efficiency by 4%. Overheating the current temperature by 10°C will
 577 improve the mean dissipation of pesticides by almost 13 %. A temperature rise of 5°C will
 578 result in a maximal mean efficiency of 67%, compared to the actual maximal dissipation rate
 579 (61%). A lower variation is noticed in the minimum pond efficiency with ascending
 580 temperatures. On average, the actual minimal dissipation rate of the AP is 30%, which is also

581 expected to rise by 4% due to a temperature increment of 5°C. On the other hand, reducing the
582 temperature by -5°C can decrease the actual efficiency by 2%.

583 **4 Discussion**

584 **4.1 Conceptual model**

585 PESTIPOND is a time-dependent model (daily-step) developed to predict the fate of pesticides
586 at the ponds' scale before being transferred to the water resources of the agricultural catchment.
587 The model is designed to be implemented in a landscape-modeling tool (e.g., SWAT (Neitsch
588 et al., 2011)) to predict pesticide behavior at the catchment scale. PESTIPOND can be
589 integrated into landscape modeling by replacing the equations of the pesticide fate sub-model
590 with PESTIPOND's formulations. Otherwise, the pesticide concentrations simulated by
591 PESTIPOND could be directly implemented as simulated data in landscape models. The
592 PESTIPOND modeling approach is built upon the mass balance of pesticides in the two main
593 compartments of AP, i.e., the water column and the active sediment layer, also designated as
594 the water-sediment interface, while considering the key physicochemical processes behind
595 pesticide behavior. PESTIPOND requires hydro-climatic input data (i.e., rainfall, PET,
596 temperature, inflow, and outflow rates) and monitoring data of the intercepted pesticides (inlet
597 concentrations).

598 The originality of the model lies in integrating and exploring the key physicochemical processes
599 to predict the export of pesticides from AP contrarily to black-box models using a single generic
600 decay coefficient. Besides, PESTIPOND uses the simplest form of mathematical formulations
601 when compared to more complex and computationally costly environmental fate models such
602 as TOXSWA and AGRO-2014 (Adriaanse, 1996; Gobas et al., 2018). Contrarily to other
603 pesticide fate models (i.e., the pond/lake module of SWAT (Neitsch et al., 2011)), PESTIPOND
604 integrates the effect of temperature and HRT as they are widely recognized as governing factors
605 of pesticide behavior in AP. Each temperature-dependent process coefficient is adjusted to the
606 actual site temperature. Plus, the processes are integrated into the model by kinetics; thus, the
607 more extended the HRT, the longer the process will have time to dissipate the molecule. In
608 contrast to SWAT, PESTIPOND integrates desorption, a considerable process for mobile and
609 hydrophilic pesticides, as underlined by the SA and mass budget results discussed afterward.

610 **4.2 Sensitivity analysis**

611 A global sensitivity analysis was performed and documented in (Bahi et al., 2023, submitted).
612 SA outcomes evidenced the insensitivity of the PESTIPOND model to hydrolysis and
613 volatilization processes. By contrast, adsorption and desorption showed the most significant
614 influence on pesticide behavior independently of their molecular properties. Similar SA
615 assumptions were made by Boulange et al. (2012) and Desmarteau and Ritter (2014) for other
616 environmental fate models. In addition, SA evidenced that the biotransformation at the water-
617 sediment interface is more effective on hydrophobic and lowly mobile pesticides, while
618 biotransformation in water is more effective on hydrophilic and highly mobile pesticides. The
619 variation of the AP efficiency with time (Fig.A. 7) can be translated by the seasonal change of
620 the impact of processes on pesticide fate. This observation fortifies the SA assumption outlining
621 that (1) the sensitivity of hydrophilic pesticides to sorption and transformation processes varies
622 with time according to the hydraulic conditions of the AP and (2) that temperature has a major
623 effect on the set of processes, particularly enhancing pesticide transformation. Afterward, the
624 model was calibrated and validated using monitoring data of 7 pesticides with contrasted

625 properties (i.e., hydrophobicity and mobility) during five periods. PESTIPOND performance
626 was graphically and statistically evaluated.

627 **4.3 Model performance**

628 For the model performance assessment, we adopted the following strategy. The performance of
629 PESTIPOND was first (i) evaluated using an annual calibration (i.e., a set of parameters proper
630 to each year (Tables A.2 & A.3) and then (ii) a generic set of parameters for all years (i.e., the
631 mean value of the annual-calibrated parameters (Table 2). Since the daily observations of
632 pesticide concentrations are not available, transformed observation data was created from bi-
633 monthly monitoring to illustrate pesticide dynamics closely. Therefore, the model performance
634 was assessed for both transformed and non-transformed observations for each step (i) and (ii).

635 Firstly, the results of steps (i) and (ii) of the performance assessment (section 5.2) proffered
636 graphical (Fig.2, Fig.3) and statistical (Tables 3 & A.4) agreements between simulations and
637 observations except for boscalid according to non-transformed observations. Given the half-
638 lives of boscalid reported in the literature (PPDB), it is biodegradable in water. Whereas
639 boscalid was stable based on the observations in the Rampillon AP (Fig A.5), which means that
640 the conditions in which the PPDB half-lives were estimated may be different from those of an
641 AP.

642 Lower KGE and NSE values were noted for step (ii) compared to (i). The drop in the
643 performance (ii) was expected since the annual calibration uses an adapted set of parameters
644 for each year (Tables A.2 & A.3), whilst a single set of parameters was used for all years
645 combined in the performance assessment (i) (Table 3).

646 Secondly, a lower KGE was noticed for all pesticides compared to the NSE values. The
647 difference between the KGE and NSE values may originate from the definition of the KGE
648 (Eq.3) based on the mean difference between simulations and observations, which puts more
649 weight on extreme values. Alternatively, the NSE (Eq.4) estimates the discrepancy between
650 observations and simulations evenly during the whole period. Given that a spike following their
651 application in the agricultural plots characterizes all the pesticide chronicles, it is anticipated
652 that the KGE will have lower values than the NSE. Notwithstanding, it is recommended to
653 evaluate model performance with more than one criterion (NSE), thus using the KGE and
654 NRMSE. Based on commonly used thresholds (Knoben et al., 2019; Moriasi et al., 2015;
655 Towner et al., 2019), the KGE and NSE values indicate a “good” model performance, except
656 boscalid, for which the model performance is considered as “not satisfactory” according to both
657 transformed and non-transformed observations. The low model performance on boscalid is also
658 portrayed by a significant discrepancy between the observed and simulated exported mass and
659 outlet concentration during 2014-2015 (Fig.A.6). Furthermore, boscalid simulations induce a
660 model relative error (36%) higher than other pesticides (<10%). Moreover, the average NRMSE
661 translates to a slight discrepancy between the observed concentrations and simulations for the
662 other pesticides.

663 Note that using the transformed observations (daily) evaluates the model's ability to simulate
664 pesticide dynamics. The non-transformed observations (bi-monthly) assess the model's capacity
665 to predict the exported fluxes and concentrations of pesticides from the AP. Therefore, based
666 on the graphical and statistical comparisons between the model outputs and both the
667 transformed and non-transformed observations while using a single set of parameters (inter-

668 annual), we assume that the PESTIPOND model is robust and able to predict the dynamics and
669 exported fluxes and concentrations of pesticides, except for boscalid, at the AP scale.

670 **4.4 Hierarchization of pesticide dissipation processes**

671 To further explore the model outcomes and confirm the SA assumptions, we closely analyzed
672 the mass budget of pesticides in the AP. We quantified the contribution of each process to
673 pesticide fate. The quantification of the mass partition of pesticides revealed that most of the
674 intercepted mass is discharged from the pond for a mean residence time of 16 days and 9 °C
675 temperature. The remaining mass is dissipated or stored in sediments and in the water column.
676 The pesticides that were mostly stored in the sediment layer are boscalid (K_{oc} (L.kg⁻¹) = 772,
677 $\log K_{ow}$ =3), chlorotoluron (K_{oc} (L.kg⁻¹) = 400, $\log K_{ow}$ =2.5), and diflufenican (K_{oc} (L.kg⁻¹) =
678 550, $\log K_{ow}$ =4.2). According to their K_{oc} and K_{ow} , these three molecules are hydrophobic (\log
679 $K_{ow} \geq 3$) and lowly mobile ($K_{oc} > 500$) (Lewis et al., 2016). Therefore, they are likely to be
680 adsorbed on sediments, which agrees with the mass budget results (Fig.5). Alternatively, the
681 pesticides manifesting a higher presence in water are mesotrione (K_{oc} (L.kg⁻¹) = 122. \log
682 K_{ow} =0.11), s-metolachlor (K_{oc} (L.kg⁻¹) = 120, $\log K_{ow}$ =2.9), bentazon (K_{oc} (L.kg⁻¹) = 55. \log
683 K_{ow} =2.34), and quinmerac (K_{oc} (L.kg⁻¹) = 86. $\log K_{ow}$ =2.7), which are hydrophilic and highly
684 mobile (Lewis et al., 2016). The results purport that PESTIPOND simulates a pesticide behavior
685 in agreement with the one expected based on their properties.

686 The PESTIPOND model was initially built to hierarchize the processes behind pesticide
687 dissipation. This hierarchization is useful for identifying the key elements to be managed in
688 order to optimize the environmental efficiency of ponds. Thus, the mass attributed to each
689 process was quantified and confronted with temperature and HRT. For all pesticides, adsorption
690 is the most significant process in pesticide behavior, except for s-metolachlor (4), which was
691 more distinguished by the transformation in the water column. By relating this result to the
692 hydrophilic and mobile properties of the pesticide, it is expected that s-metolachlor undergoes
693 limited adsorption, which increases its bioavailability for transformation in the water column
694 than the sediment layer. A similar observation was made for s-metolachlor by (Droz et al.,
695 2021) based on laboratory experiments. By contrast, more significant adsorption was detected
696 for the hydrophobic boscalid, chlorotoluron, and diflufenican (Fig.5), followed by a
697 transformation in the sediment layer. In fact, the significant adsorption of hydrophobic
698 pesticides was heavily evidenced in the literature (Hand et al., 2001; Tang et al., 2017; Vagi
699 and Petsas, 2022) based on their high affinity to the organic carbon of sediments and
700 hydrophobicity translated by a high K_{oc} and $\log K_{ow}$, respectively. Boscalid, chlorotoluron,
701 and diflufenican are more likely to be adsorbed on sediments and thus are more bioavailable
702 for biotransformation at the water-sediment layer, contrarily to more hydrophilic and mobile
703 pesticides. For instance, bentazon, s-metolachlor, and quinmerac being hydrophilic and highly
704 mobile, are more likely to be transformed in water (Table A.6). This result underlines the link
705 between adsorption and pesticide bioavailability for biotransformation as suggested by previous
706 experimental studies (Ahmad et al., 2004; Budd et al., 2011; Chaumet et al., 2021; Lee et al.,
707 2004; Mulligan et al., 2016). The low $\log K_{ow}$ (<3) of bentazon, mesotrione, and quinmerac
708 indicate that they are likely to be re-mobilized from the sediment, which was reflected by the
709 mass budget detecting a desorption flux for all monitoring periods. For hydrophilic and highly
710 mobile pesticides, desorption covered a non-negligible part of the intercepted mass.

711 On average, for all pesticides and periods combined, adsorption covers 22% of the input mass,
712 followed by 10% for biotransformation in water and desorption with 6%, leaving 5% for
713 biotransformation and the water-sediment interface. Photolysis covers a negligible part of the
714 total transformation in water (< 1%), except for bentazon ($\approx 8\%$). However, when looking at
715 pesticides separately, hydrophobic and lowly mobile pesticides had higher biotransformation at
716 the water-sediment interface than in the water. The mass budget results support the significance
717 of adsorption, desorption, and biotransformation in the water for hydrophilic and mobile
718 pesticides. Alternatively, biotransformation at the water-sediment interface is more pronounced
719 and, desorption is limited for hydrophobic and lowly mobile pesticides.

720 SA results contended that adsorption is the most influencing process of pesticide behavior,
721 fortifying the mass budget results showing that an important fraction of the intercepted mass
722 was adsorbed for most pesticides. The mass budget also exhibited a higher transformation in
723 water and desorption effect on hydrophilic and mobile pesticides, explaining why these types
724 of molecules were more sensitive to processes occurring in the water column. Conversely,
725 hydrophobic and lowly mobile pesticides were distinguished by higher adsorption and
726 transformation in the active sediment layer, which is in line with the SA outcomes displaying a
727 higher sensitivity to processes occurring at the water-sediment interface for this kind of
728 pesticides. Combining the model results and SA outcomes, we assume that adsorption-
729 desorption and biotransformation are major processes behind pesticide fate. Hydrophobic and
730 lowly mobile pesticides are more likely to be biotransformed in the active sediment layer than
731 in water. At last, volatilization and hydrolysis have a negligible contribution to pesticide
732 dissipation.

733 **4.5 Dissipation efficiency and pond properties**

734 In addition, the PESTIPOND model enables the assessment of the link between pesticide
735 dissipation and pond properties (i.e., temperature and HRT). The mass budget results (Fig.4)
736 highlighted a higher transformation of bentazon, boscalid, and s-metolachlor 2016-2017,
737 characterized by the highest mean temperature (12°C) and HRT (28 days). Also, bentazon,
738 diflufenican, and s-metolachlor underwent higher adsorption during 2019-2020, having a
739 higher HRT (27 days). The same pesticide had a lower transformation during 2018-2019,
740 characterized by a lower mean temperature (8°C). Moreover, the desorption of bentazon and
741 mesotrione was more significant during 2018-2019, when the HRT was only 8 days.

742 These results support the link between temperature, HRT, and pesticide behavior. Higher
743 temperatures enhance the microbial activity behind the biotransformation and are accompanied
744 by important solar radiations, which favors photolysis (Kaur and Vishnu, 2022; Law et al.,
745 2014; Motoki et al., 2020; Rani and Sud, 2015). Therefore, significant pesticide transformation
746 was noticed during periods of high temperature. In addition, higher HRT provides a longer time
747 for pesticides to be adsorbed and transformed. Similarly, for some pesticides higher desorption
748 was noted during low-HRT periods while it was the opposite for other pesticides. This result
749 suggests that no direct link between desorption and HRT was noticed.

750 The link between temperature, HRT, and pesticide dissipation raises concerns about the impact
751 of pesticides' application period. For instance, except for chlorotoluron, the set of pesticides is
752 applied in spring, which tends to have significant rainfall events. Therefore, during spring,
753 pesticides are more likely to be intercepted by the AP due to runoff following rainfall events
754 and thus be dissipated by the synergy of the above-described processes. Moreover, spring-

755 applied pesticides are more susceptible to transformation as the temperatures rise. Although
756 this is also the case for summer-applied pesticides, it is unlikely that these chemicals will get to
757 the pond due to limited rainfall events. Alternatively, pesticides applied during winter and
758 autumn, such as chlorotoluron, even though intercepted by the AP, their transformation is less
759 expected due to the weak microbial activity associated with cold temperatures. This assumption
760 could explain the mass budget result illustrating a lower transformation of chlorotoluron, which
761 is applied during autumn and winter in Rampillon. By contrast, spring and summer-applied
762 pesticides (i.e., bentazon, mesotrione, and s-metolachlor) were more favorable to
763 transformation in the water column (Table A. 6). The model extrapolation results evidenced
764 that a temperature rise of 10°C will increase the mean dissipation potential of the AP by 13%
765 (Fig.A.9). In comparison, a temperature drop of 5°C decreases the efficient by only 2%. These
766 results provide insight into the geographical variation of AP efficiencies between warm and
767 cold areas.

768 Besides low temperatures, winter and autumn-applied pesticides face strong flows that reduce
769 their residence time in the pond to undergo the different dissipation processes. Therefore, to
770 remediate this issue, the surface area of the AP can be enlarged to increase the HRT and, thus
771 the residence time of pesticides. Accordingly, an estimation of the AP efficiencies according to
772 ascending surface areas (Fig.6) was performed. The results showed that once the AP covers
773 >1% of the drained catchment area, the dissipation of pesticides reaches 84%, which is almost
774 twice and a half of the actual efficiency of the Rampillon AP. [Tournebize et al. \(2012\)](#) reported
775 that, based on a literature review of AP performances, scientists suggested allocating 1% of the
776 catchment area to the pond. However, farmers rejected this proposal for different reasons (land
777 occupation, cost, operational labor cost, and maintenance). Consequently, the farmers
778 suggested a 0.15% area for the AP to meet their requirements or acceptability, which was
779 expected to be a less efficient remediation solution for pesticide transfer. The PESTIPOND
780 simulations, predicting a significantly higher efficiency of the AP if it covers 1% of the
781 catchment, supported this expectation. In addition, the extrapolation results evidenced that the
782 HRT has a significantly higher impact on the AP efficiency when compared to the temperature
783 rise. This assertion was expected since the HRT drives the efficiency of all processes, namely
784 adsorption, desorption, and transformation, while temperature only influences transformation
785 processes. This assumption is supported by the mass budget results, indicating a higher
786 transformation of pesticides during high-HRT periods (2016-2017) even though the
787 temperature is low. In addition, adsorption is a major dissipation process occurring mainly at
788 the water-sediment interface. Hence, increasing the HRT by increasing the AP area is
789 equivalent to increasing the water-sediment interface where pesticide retention occurs. This
790 explains the higher efficiency in larger ponds and the major role of the water-interface sediment
791 in pesticide dissipation.

792 From another viewpoint, adsorption can be a concern over the long term as it accumulates
793 pesticides in the sediment. However, recent in-situ measurements of pesticide concentrations
794 in the Rampillon AP sediments showed that after ten years, only a few amounts of pesticides
795 were accumulated (<7ng.g⁻¹). Moreover, another in-situ experiment was performed in
796 mesocosms, evidenced that bentazon was the only pesticide sensitive to light, which supports
797 the model result indicating a significant photolysis of the molecule in question.

798 **4.6 Calibrated parameters and pesticide properties**

799 The parameter set used for this model validation was compared to literature values. Due to the
800 non-availability of adsorption-desorption parameters, k_{ads} and k_{des} were calibrated. The
801 obtained values were in the order of magnitude of similar studies' calibrated parameters
802 (Comoretto et al., 2008; Nakano et al., 2004; Watanabe et al., 2006; Yoshida and Nakano,
803 2000). In addition, a strong correlation ($R^2=0.9$) between k_{ads} and K_{oc} was noticed, except for
804 s-metolachlor (Fig.A.7). A first correlation equation was defined for mobile pesticides ($K_{oc} <$
805 120 L.kg^{-1}) and a second one for lowly mobile pesticides ($K_{oc} > 300 \text{ L.kg}^{-1}$). For mobile
806 pesticides, the desorption parameter can be deduced from the adsorption kinetic and set to zero
807 for lowly mobile molecules. Transformation parameters ($DT_{50,w}$, $DT_{50,s}$, and $DT_{50,p}$) were
808 extracted from the PPDB (Lewis et al., 2016), and some were calibrated to improve the model
809 performance (Table 2). The calibrated parameters were $DT_{50,w}$ and $DT_{50,s}$ for 4 pesticides out
810 of 7. Globally, the calibrated half-lives were shorter than the PPDB values. In water, the
811 dissipation was, on average, 75, 7, and 80 days faster for bentazon, s-metolachlor, and
812 quinmerac, respectively, than in the laboratory (i.e., where the PPDB values are estimated). In
813 the water-sediment interface, the dissipation was, on average, 600 and 8 days faster for bentazon
814 and chlorotoluron, respectively. This result indicates a faster dissipation under field conditions
815 than in laboratory experiments. The same assumption was made by Bahi et al. (2023b),
816 suggesting that pesticides face a single process in laboratory experiments (PPDB).
817 Contrastingly, pesticides undergo a synergy of on-site processes that enhance their dissipation
818 owing to a shorter half-life. Boscalid was the only pesticide having a calibrated $DT_{50,w}$ (500
819 days), a hundred times longer than the PPDB value (5 days), which may explain the low model
820 performance according to this molecule. However, other sources substantiate the belief that
821 boscalid is stable in water and sediments and is rather adsorbed on sediments (Keith and
822 Walker, 1992; Mergia et al., 2022), assisting the mass budget results (Fig.4).

823 **4.7 PESTIPOND limitations**

824 The strong foundation on which this model is built is represented by the numerous results
825 of pesticides with contrasting properties and application periods. However, the limitations of
826 PESTIPOND should be recognized. First, the assumption of a completely mixed reactor is not
827 always the case in APs, specifically those representing heterogeneities (i.e., significant
828 vegetation cover, dikes, and dead zones). Therefore, the PESTIPOND model could be
829 complemented if coupled with hydraulic-based models, such as 3D or 2D models (Lemaire et
830 al. (2022), *under review*). 3D computational fluid dynamics models incorporate relevant pond
831 compartments (plant/water and sediment/plant interfaces). However, these compartments may
832 require excessive computation time (Tsavdaris et al., 2013). Therefore, 2D models are a better
833 alternative, as they are less computationally costly and include explicitly the vegetation patches
834 to estimate the water pathways and their transit times in ponds (Imfeld et al., 2021; Silva and
835 Ginzburg, 2016). Secondly, considering microbial communities' acclimation and dynamics will
836 undoubtedly improve the model's performance. The model prediction could also be expounded
837 by considering the fate of transformation products. Additionally, if the model integrates the
838 dynamics of organic carbon content, the adsorption-desorption effect would be better
839 expounded.

840 The model was validated for bi-monthly observations of pesticides. Yet, the accuracy of
841 PESTIPOND validation can be ameliorated if daily observations of pesticides were available.
842 Notwithstanding, the model is robust and simulates a pesticide behavior close to observations

843 and the one expected based on molecular properties. In addition, PESTIPOND is a readily
844 configurable model since the transformation parameters can be inspired from literature (PPDB)
845 and adsorption-desorption parameters deduced from the pesticide property K_{oc} . Furthermore,
846 the originality of PESTIPOND lies in the ability to predict pesticide partition in AP and quantify
847 the contribution of each physicochemical process to their overall behavior while integrating
848 temperature and HRT effects.

849 **5 Conclusion**

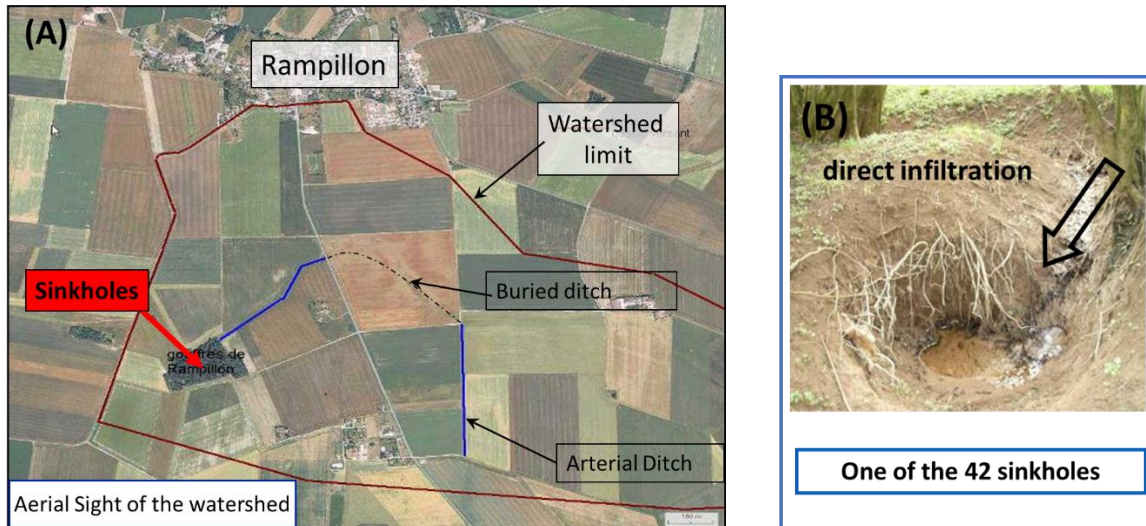
850 PESTIPOND is a process-based model developed to predict the fate of pesticides in APs. The
851 model is designed to be integrated into landscape agro-hydrological modeling tools to
852 extrapolate the prediction to the catchment scale.

853 The key assumptions to be drawn from this study are (i) that adsorption-desorption and
854 transformation are governing processes in pesticide fate. (ii) Hydrophobic and lowly mobile
855 pesticides are more likely to be transformed at the water-sediment interface. Although the fate
856 of the transformation products is still unknown, the exported amount of mother pesticide
857 molecules will be dissipated before reaching natural water resources. (iii) Hydrophilic
858 pesticides, despite being less retained in APs, can be subjected to transformation in the water
859 column, especially during summer and spring, when temperature arises. A higher HRT will
860 increase the dissipation probability for both hydrophilic and hydrophobic pesticides in the water
861 column. Longer HRT provides more time for pesticides to be adsorbed and transformed within
862 the AP. Accordingly, the PESTIPOND model predicted that the actual efficiency of the AP
863 covering 0.15% of the drained catchment would double if the pond's surface area covered at
864 least 1% of the catchment. By contrast, the model's predictions evidenced that a temperature
865 rise of 10°C will increase the dissipation of pesticides by only 8%. It is noteworthy that a
866 temperature rise entails a more significant transformation and hence more transformation
867 products. However, the model does not consider these latter, which can be addressed later by
868 adding a transformation products compartment to predict its fate in APs.

869 Given that, we assume that PESTIPOND provides key elements that are useful to design and
870 manage ponds with optimal efficiency. Hence, these ponds can be complementary solutions to
871 pesticide use regulation to reduce the transfer of agricultural contamination into the
872 environment. PESTIPOND can be implemented afterward in landscape modeling tools to
873 extrapolate the prediction of pesticide behavior from the pond scale to the catchment scale.

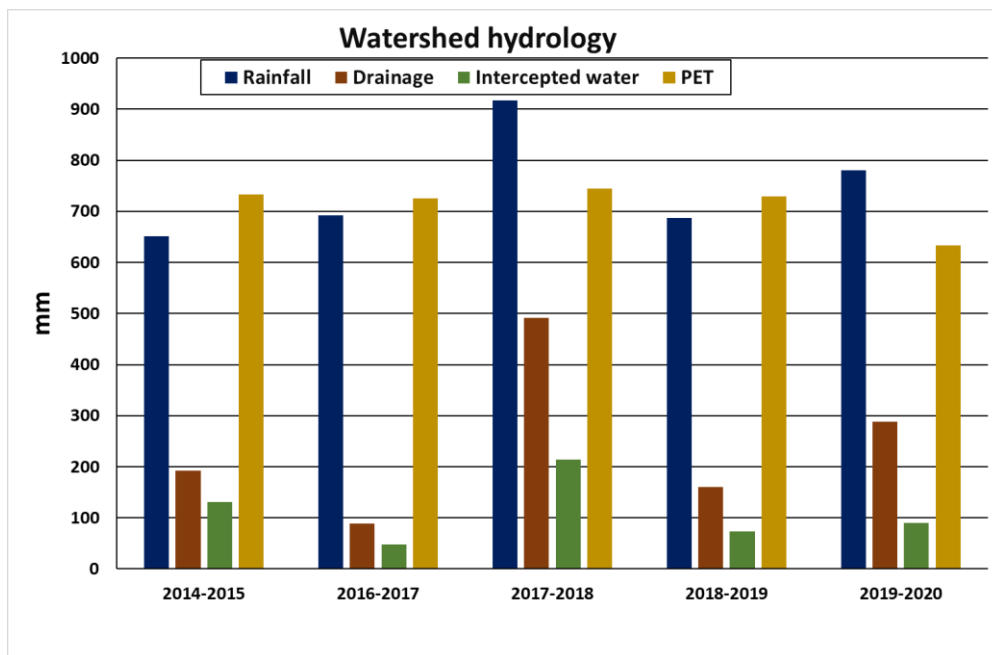
874 **6 Appendix**

875 **6.1 Properties of the Rampillon AP**



876

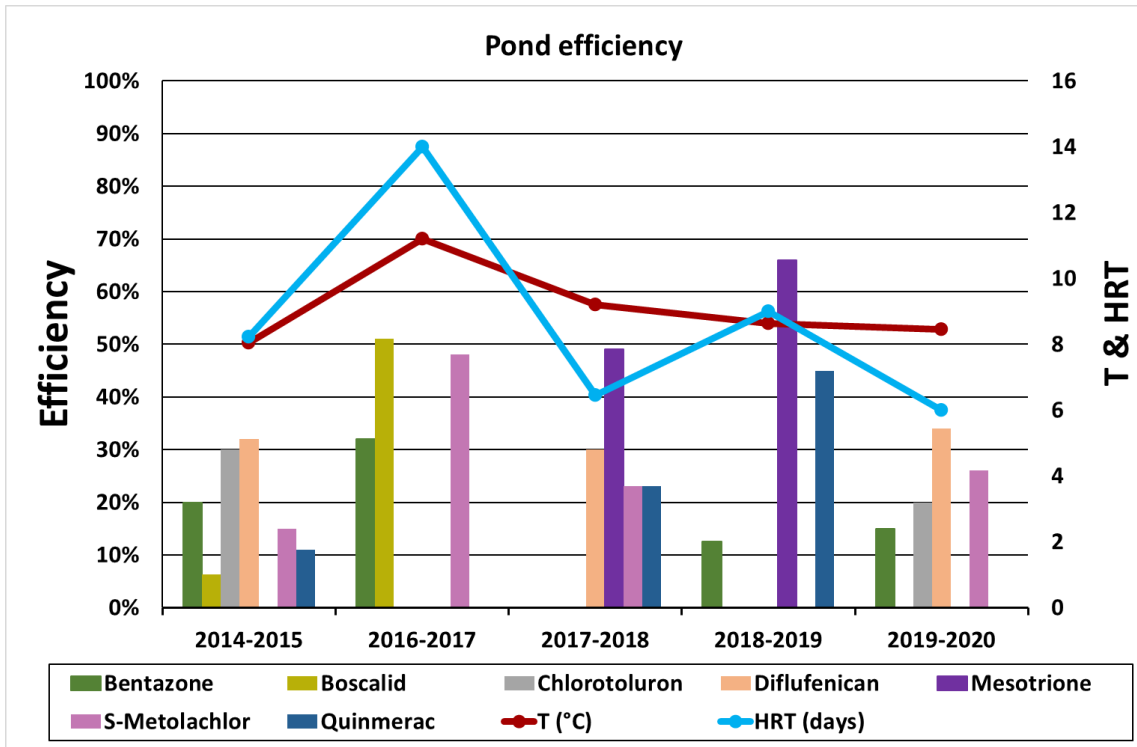
877 **Figure A.1:** Aerial sight of the Rampillon watershed (355 ha) (A). The watershed comprises two arterial ditches
 878 (blue lines) and a buried ditch (dashed line). The red arrow points toward sinkholes. Fig.A.1 (B) displays one of
 879 the 42 sinkholes contained in the watershed.



880

881 **Figure A.2:** Summary of hydrological inputs of the 355-ha watershed where the Rampillon AP is implemented.
 882 The blue bars represent the local rainfall, the brown bars represent the drained water in the watershed, the green
 883 bars represent the total intercepted water by the AP, and the gold bars display the local PET estimated by the Oudin
 884 formula (ref). The hydrological inputs (mm) are calculated from the total volume (m³), which is normalized by the
 885 watershed area (355 ha).

886



888

889 **Figure A.3:** Percentage of the mean efficiency of the Rampillon AP to reduce the concentration between the inlet
 890 and outlet (bars) of the studied pesticides. The red line represents the mean temperature T (°C) of each period and
 891 the blue line refers to the mean hydraulic residence time HRT (d) in the AP. The data is displayed according to the
 892 periods used for model validation.

893

894 **6.2 Model inputs**

895

896 **Table A.1:** List of the PESTIPOND model variables and parameters. The details on how the input data is
 897 obtained are available in (Bahi et al. 2023. submitted).

Values	Parameters	Symbol	Units
Literature/PPDB	Biotransformation in the active sediment layer	$k_{bio,s}$	T^{-1}
	Photolysis	k_p	T^{-1}
	Hydrolysis	k_h	T^{-1}
	Henry constant	H	$Pa.m^3.mol^{-1}$
	Gas constant	R	$Pa.m^3.mol^{-1}.K^{-1}$
	Mass transfer coefficient of CO ₂ in water	k_{CO_2}	$M.T^{-1}$
	Mass transfer coefficient of HO ₂ in water	k_{H_2O}	$M.T^{-1}$
	Molecular weight of CO ₂	MW_{CO_2}	Mol
	Molecular weight of HO ₂	MW_{H_2O}	Mol
	Molecular weight of the pesticide	MW	Mol
	Temperature factor	θ	Unitless
On-site measurements	Surface area of the AP	A	L^2
	Bulk density of the sediment layer	ρ_b	$M.L^{-3}$
Calibration	Adsorption kinetic coefficient	k_{ads}	T^{-1}
	Desorption kinetic coefficient	k_{des}	T^{-1}
PPDB/Calibration	Biotransformation in water	$k_{bio,w}$	T^{-1}
Forcing functions/External variables			
On-site measurements	Inlet concentration of the pesticide	$C_{in}(t)$	$M.L^{-3}$
	Inflow rate	$Q_{in}(t)$	$L^3.T^{-1}$
	Water depth	$h_w(t)$	L
	Temperature	T(t)	°C
	Rainfall	P(t)	L
	Evapotranspiration	PET(t)	L
	Outflow rate	$Q_{out}(t)$	$L^3.T^{-1}$
Hydrological model	Water depth	$h_w(t)$	L
	Water volume	$V_w(t)$	L^3
State variables			
Model outputs	Pesticide mass in the water	$M_w(t)$	M
	Pesticide mass in the active sediment layer	$M_s(t)$	M

898

899

900 **Table A.2:** Values of the model parameters related to adsorption and desorption for the 20 study cases. k_{ads} (d^{-1})
 901 and k_{des} (d^{-1}) are the adsorption and desorption kinetic coefficients, respectively. These values are the result of the
 902 annual calibration of the parameters. The set of adsorption and desorption values for the selected pesticides were
 903 calibrated because no available data was found of the literature. The calibrated values fit in the range of other
 904 studies (Comoretto et al., 2008; Nakano et al., 2004; Watanabe et al., 2006; Yoshida et al., 2000). These values
 905 are the result of the annual calibration of the parameters.

Pesticides	2014-2015		2016-2017		2017-2018		2018-2019		2019-2020		PPDB	
	k_{ads}	k_{des}	k_{ads}	k_{des}	k_{ads}	k_{des}	k_{ads}	k_{des}	k_{ads}	k_{des}	Koc	log Kow
Bentazone	0.19	0.015	0.2	0.015	-	-	0.11	0.015	0.11	0.015	55	2.34
Boscalid	0.06	0	1.2	0	-	-	-	-	-	-	772	3
Chlorotoluron	0.15	0	-	-	-	-	-	-	0.7	0	400	2.5
Diflufenican	0.26	0	-	-	0.27	0	-	-	1	0	550	4.2
Mesotrione	-	-	-	-	0.08	0.01	1.3	0.1	-	-	122	0.11
S-Metolachlor	0.08	0.01	0.08	0.01	0.08	0.01	-	-	0.06	0.01	120	2.9
Quinmerac	0.03	0.012	-	-	0.03	0.012	1.25	0.03	-	-	86	2.7

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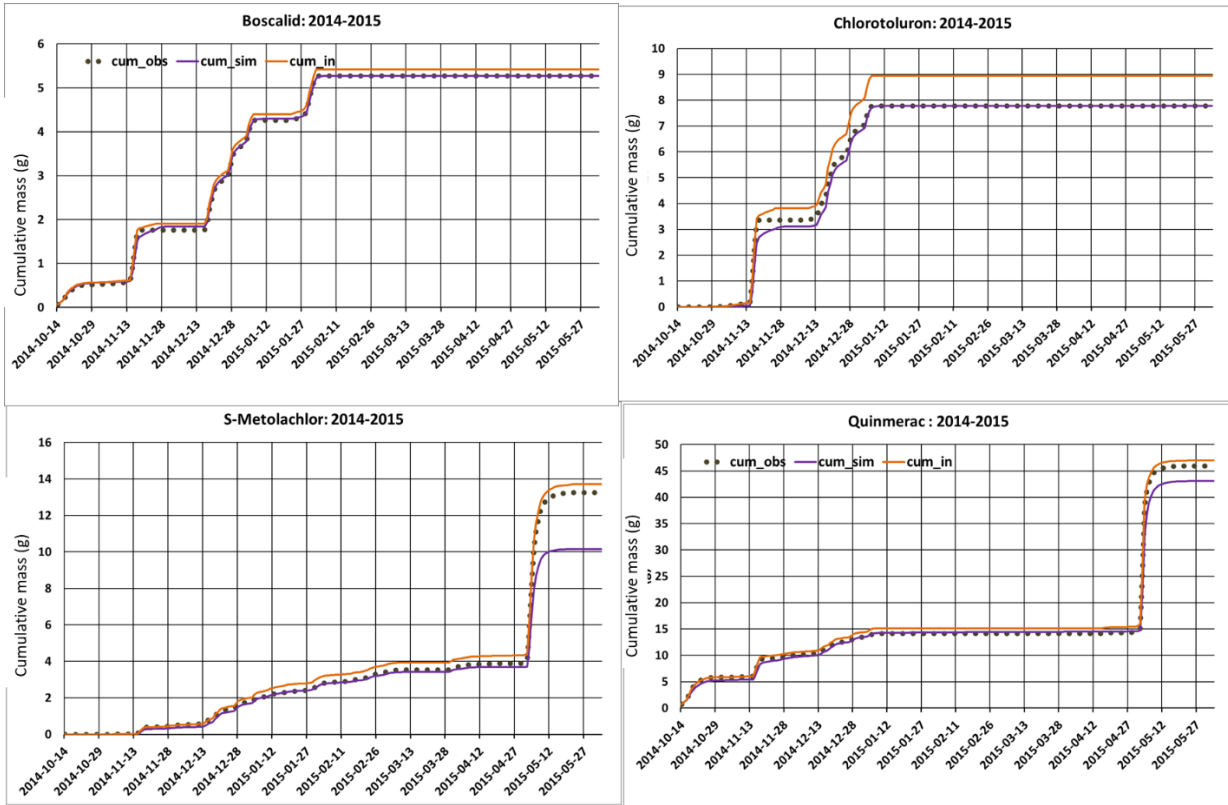
907 **Table A.3:** Values of the model parameters related to transformation processes, i.e., $DT_{50,w}$ (d), $DT_{50,s}$ (d), and
 908 $DT_{50,p}$ (d), are the biotransformation in water, in the active sediment layer, and the photolysis half-lives,
 909 respectively. Most of transformation parameters were extracted from the PPDB and (*) are the calibrated values.
 910 Similarly to adsorption-desorption parameters, these values are the result of the annual calibration of the
 911 parameters.

Pesticides	2014-2015			2016-2017			2017-2018			2018-2019			2019-2020		
	$DT_{50,w}$	$DT_{50,s}$	$DT_{50,p}$	$DT_{50,w}$	$DT_{50,s}$	$DT_{50,p}$	$DT_{50,w}$	$DT_{50,s}$	$DT_{50,p}$	$DT_{50,w}$	$DT_{50,s}$	$DT_{50,p}$	$DT_{50,w}$	$DT_{50,s}$	$DT_{50,p}$
Bentazon	5	100	3	5	100	3	-	-	-	5	100	3	5	100	3
Boscalid	500*	500	stable	500*	500	stable	-	-	-	-	-	-	-	-	-
Chlorotoluron	44	300	30	-	-	-	-	-	-	-	-	-	1*	300	30
Diflufenican	200	175	133	-	-	-	200	175	133	-	-	-	200	175	133
Mesotrione	-	-	-	-	-	-	5,3	5,2	89	5,3	5,2	89	-	-	-
S-Metolachlor	1,5	43	146	1,5	43	146	1,5	43	146	-	-	-	1,5	43	146
Quinmerac	5	180	66	-	-	-	1,5*	180	66	5	180	66	-	-	-

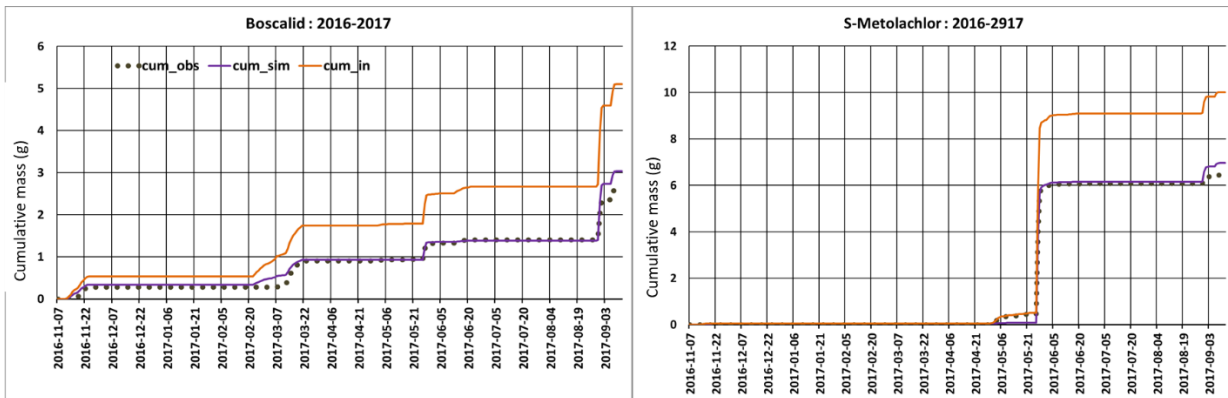
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914 **6.3 Outputs of the periodic calibration**

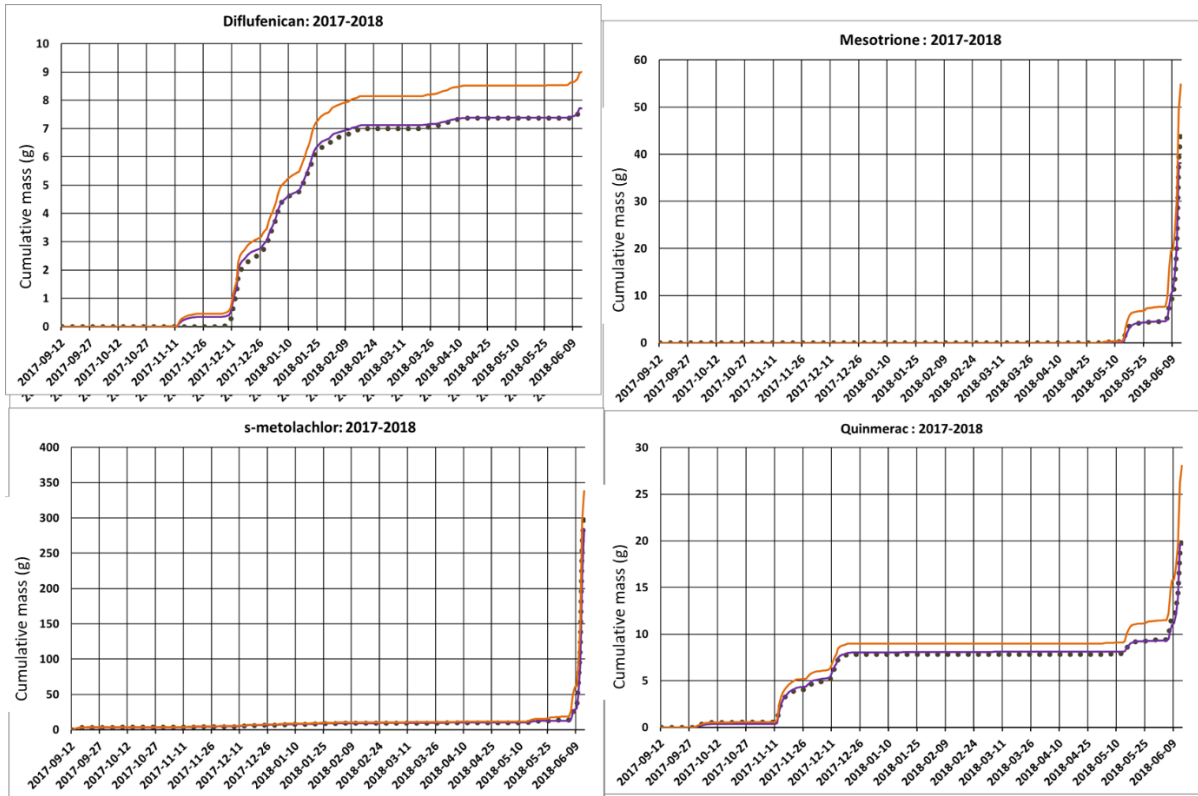


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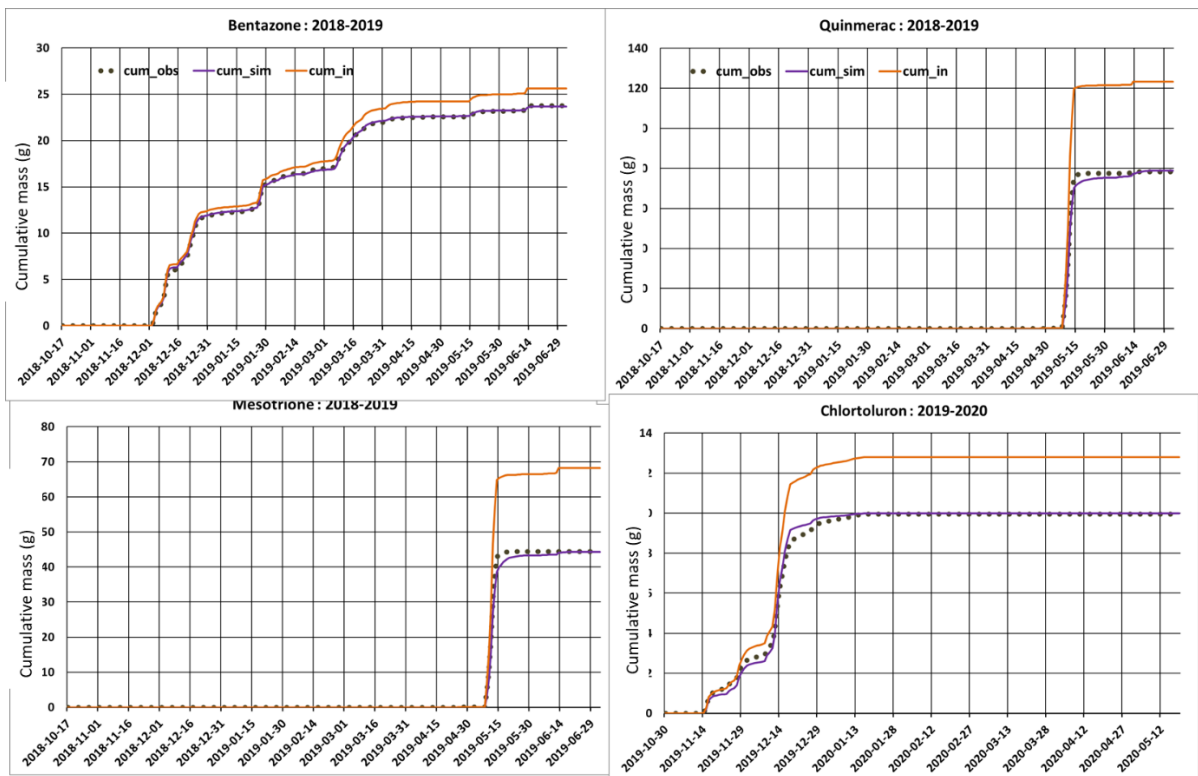


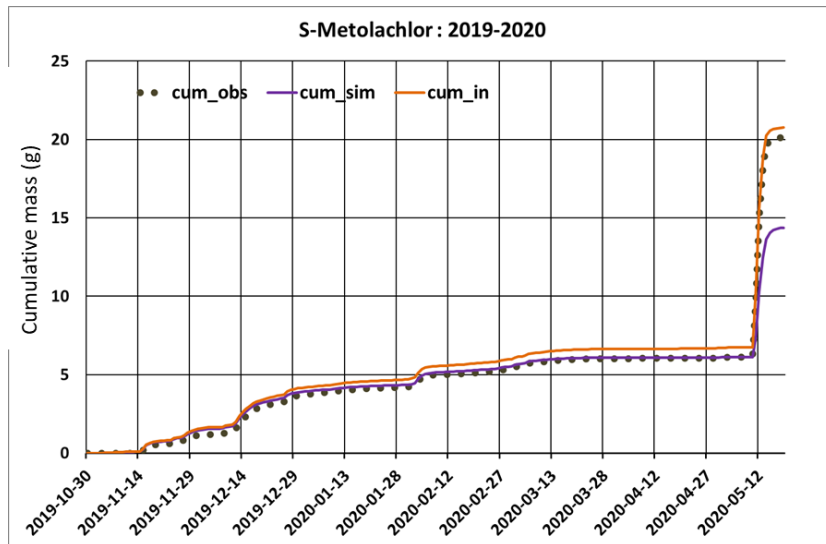
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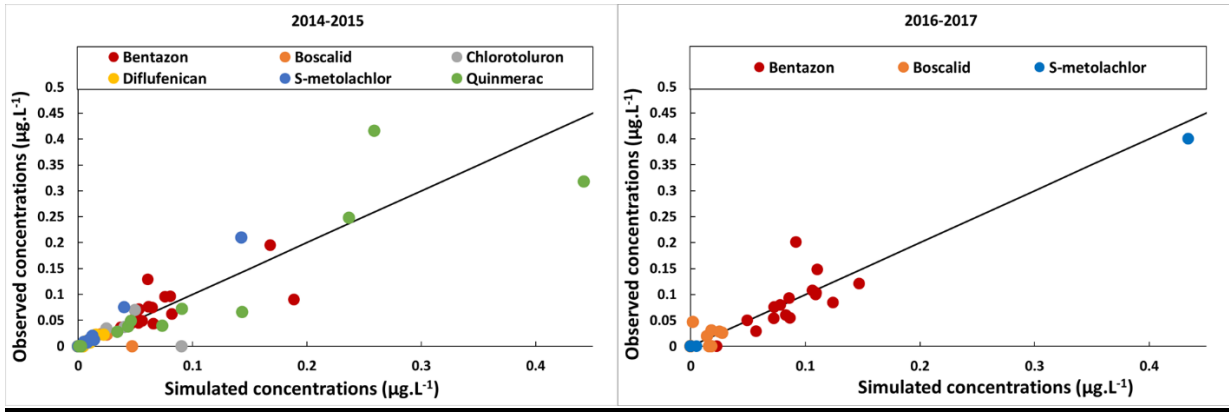


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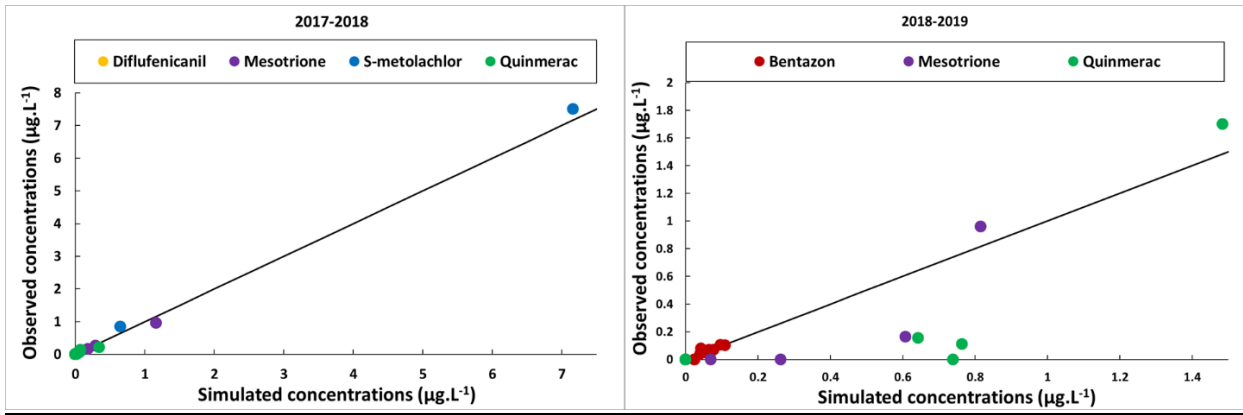
920 **Figure A.4:** Graphical comparison of simulated (purple lines) and observed (dark points) cumulative masses of
 921 the pesticides monitored during 2019-2020 in the outlet and the corresponding cumulative influx mass (orange
 922 line). cum_obs cum_sim are the cumulative masses of the observations and simulations of pesticide mass at the
 923 AP outlet using annual calibration. cum_in is the cumulative mass of the observed pesticide mass at the AP inlet.
 924 The corresponding KGE, NSE, and NRMSE are listed in Table 3.

925

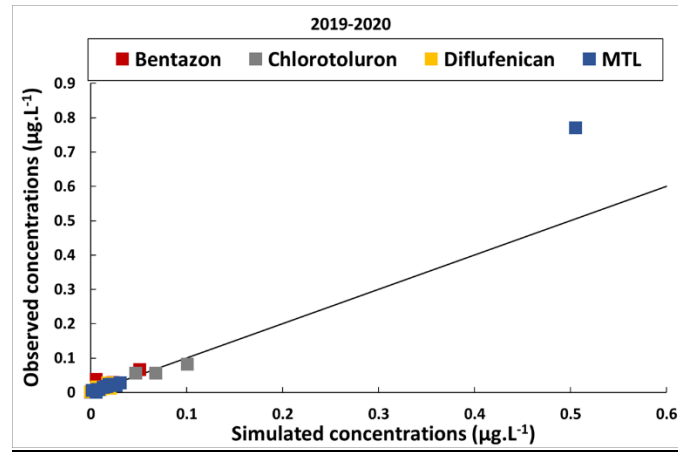
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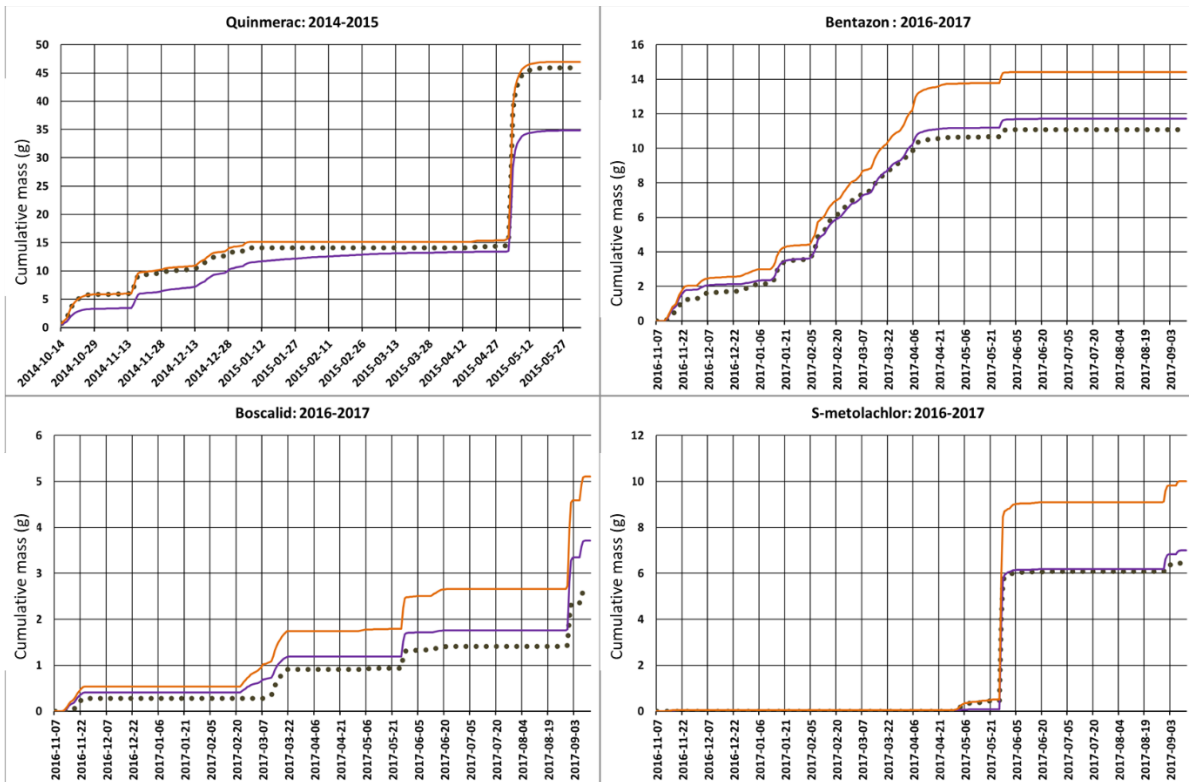
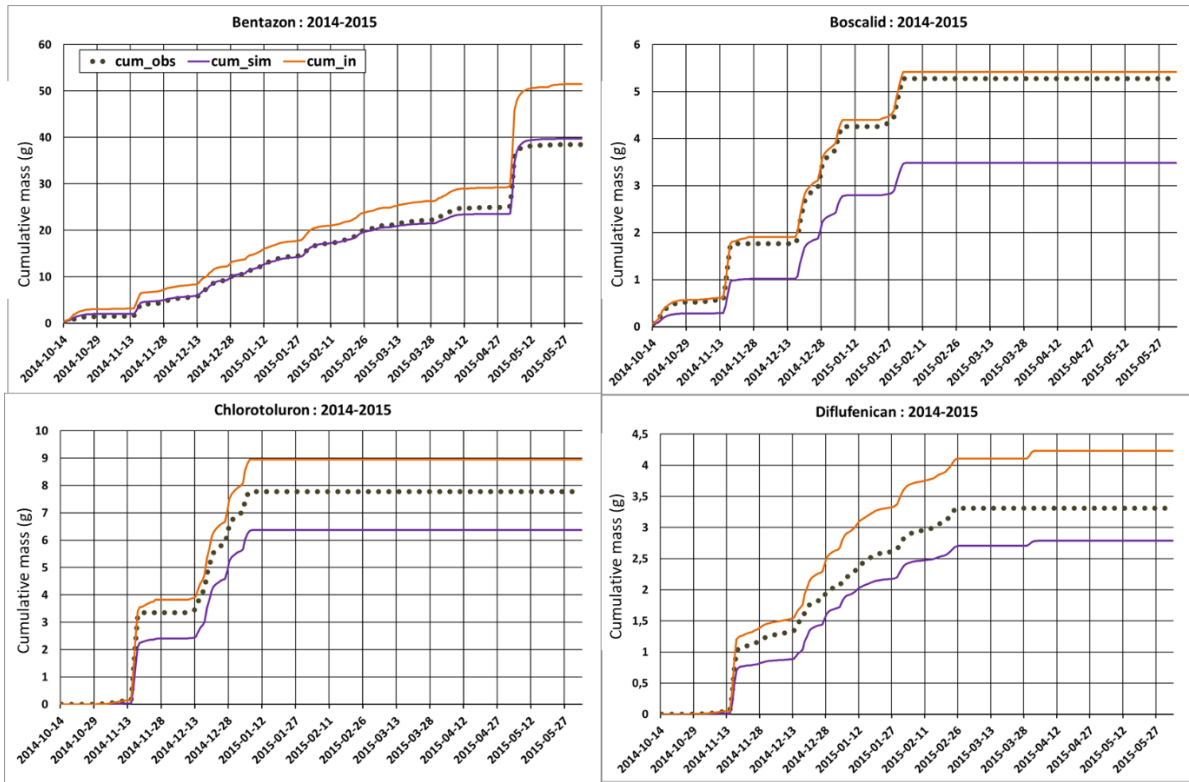


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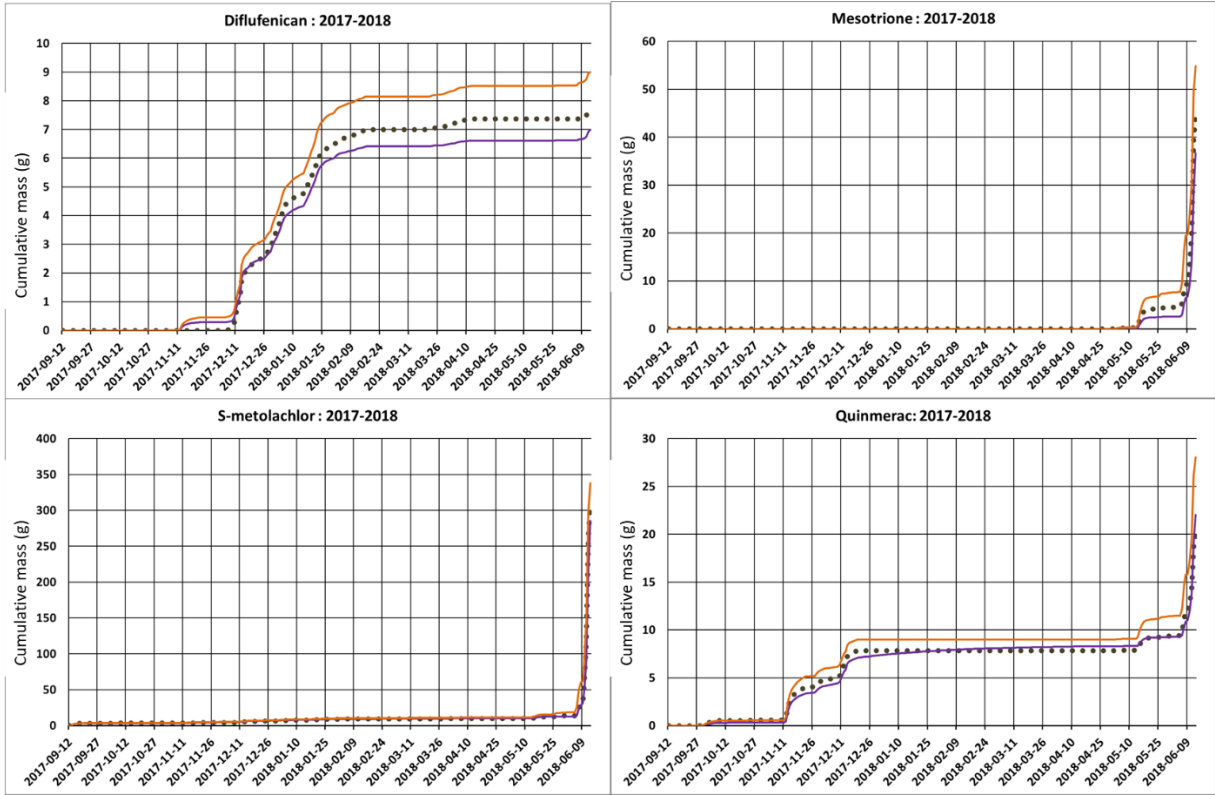


929 **Figure A.5:** Graphical comparison of the bi-monthly observations (y-axis) and simulations (x-axis) of all pesticide
930 outlet concentrations ($\mu\text{g.L}^{-1}$) and periods combined, using the annual calibration. Each color points out a specific
931 pesticide. The black line in the middle refers to simulations equal to observations ($y=x$).

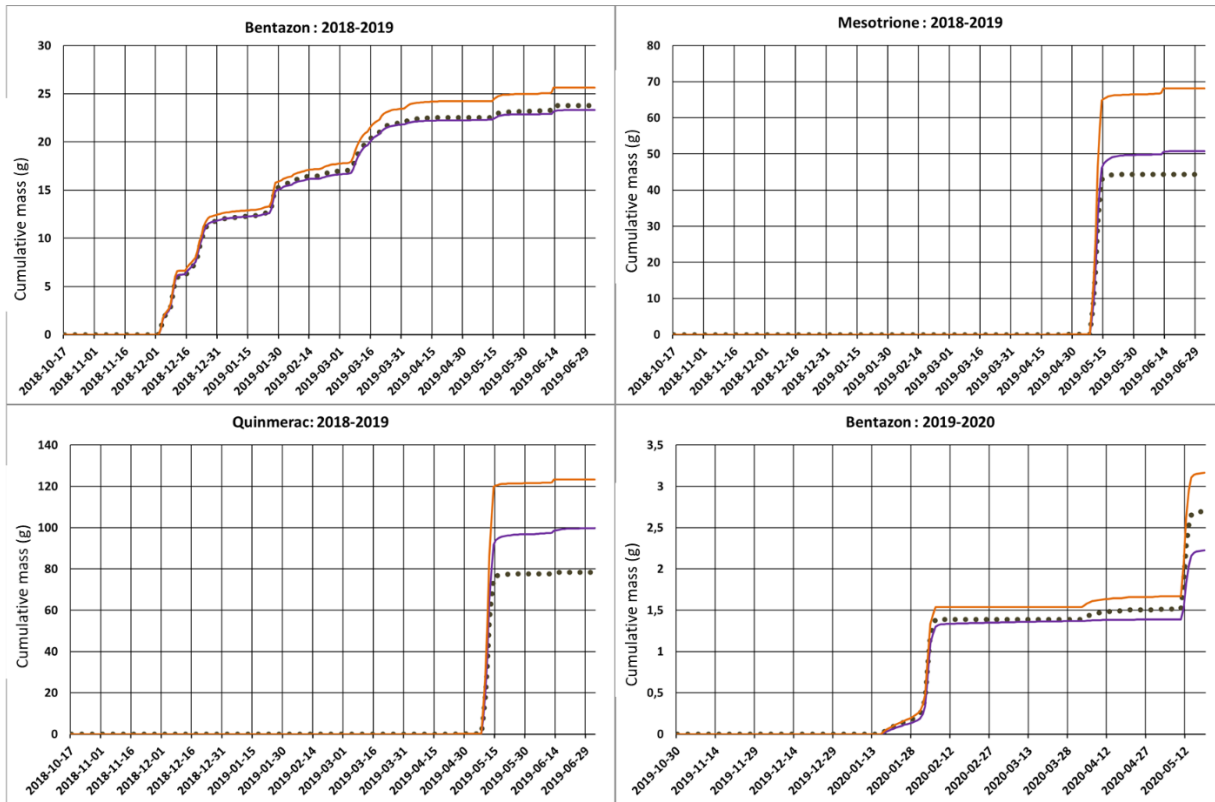
6.4 Outputs of the calibration with the mean set of parameters

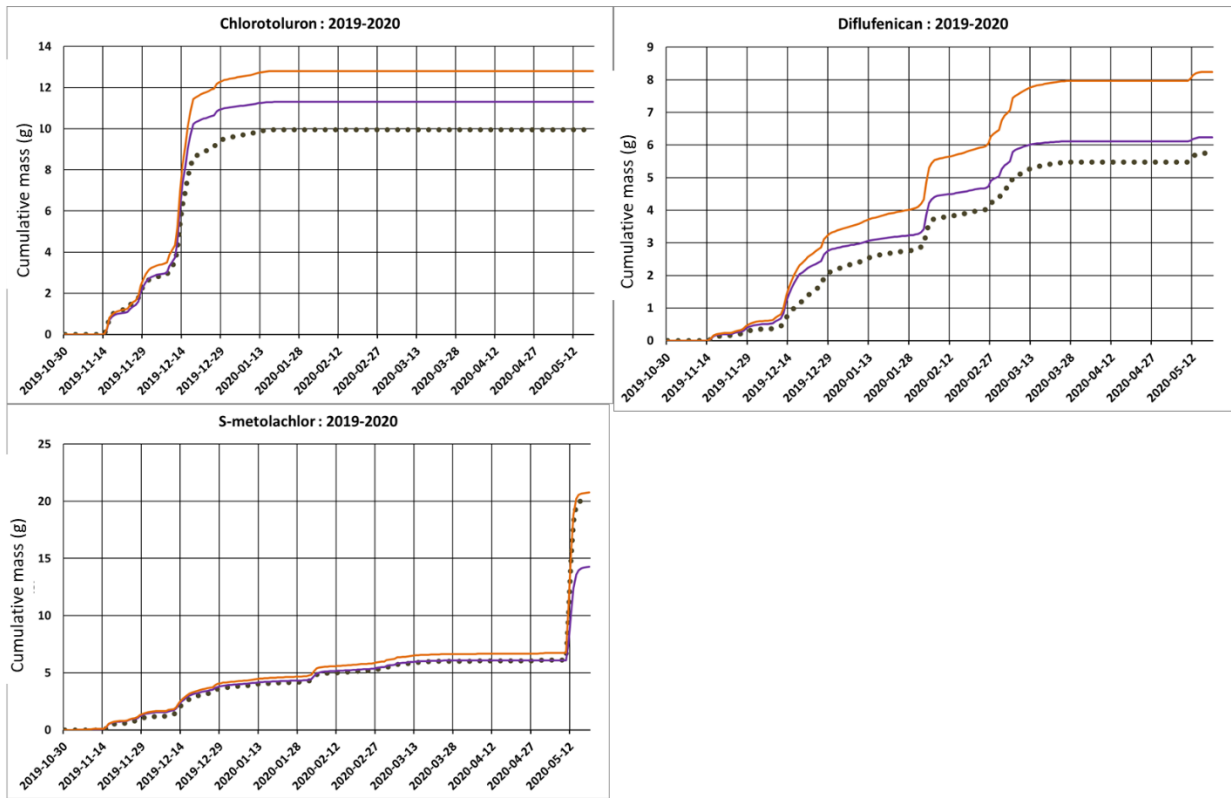


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938 **Figure A.6:** Graphical comparison of simulated (purple lines) and observed (dark points) cumulative masses of
 939 pesticides in the outlet and the corresponding cumulative influx mass (orange line) for all pesticides and periods
 940 combined. The corresponding KGE, NSE, and NRMSE are listed in Table 3.

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942 6.5 Statistical tests

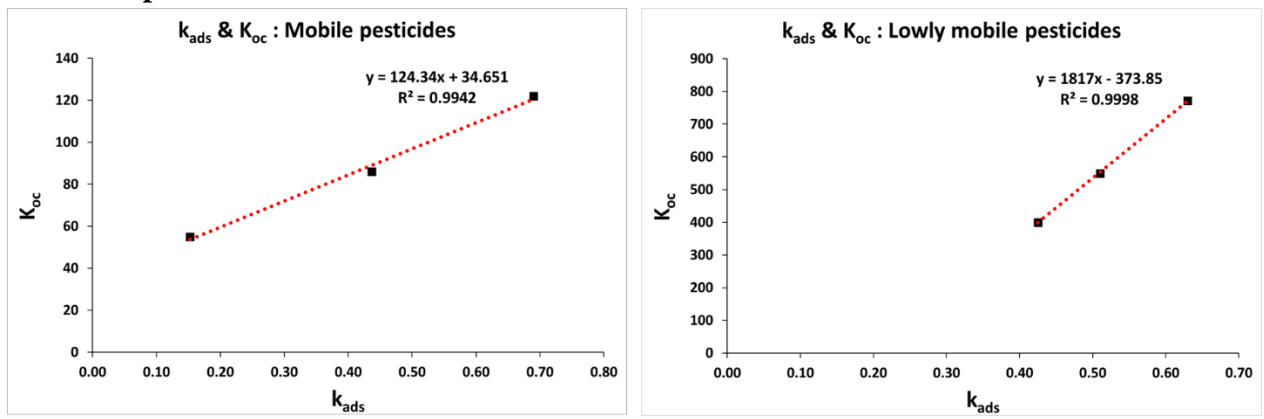
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944 **Table A.4:** Results of the statistical tests.

Test	2014-2015	2016-2017	2017-2018	2018-2019	2019-2020
Student's test	<i>t-value</i> : 0.40	<i>t-value</i> : 0.1	<i>t-test</i> : 0.11	<i>t-test</i> : -0.30	<i>t-test</i> : 0.18
	<i>p-value</i> : 0.68	<i>p-value</i> : 0.76	<i>p-value</i> : 0.87	<i>p-value</i> : 0.72	<i>p-value</i> : 0.81
Regression	R ² : 0.76	R ² : 0.41	R ² : 0.78	R ² : 0.85	R ² : 0.87
	<i>p-value</i> : 7.3E-04	<i>p-value</i> : 0.01	<i>p-value</i> : 1E-08	<i>p-value</i> : 2.3E-03	<i>p-value</i> : 2.7E-04

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946 **6.6 Sorption coefficients**



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948 **Figure A. 7** Linear correlation between the calibrated adsorption parameter (k_{ads}) and the mobility (K_{oc}) of
949 pesticides (extracted from the PPDB (Lewis et al., 2016)). The left graph illustrates the correlation for mobile
950 pesticides (low K_{oc}) and the right graph displays the correlation for lowly mobile pesticides (high K_{oc}).

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954 **6.7 Pesticide mass budget**

955 **Table A.5:** Summary of the mass budget (g) for the studied pesticides. M_T is the total mass of the pesticide at the
 956 end of each period. M_w and M_s are the pesticide masses in water and sediments at the end of each period.
 957 respectively. $\sum M_{in}$ is the total intercepted mass. $\sum M_{out}$ the total mass discharged from the pond and $\sum M_{tr}$ is the
 958 total transformed mass. $\sum M_{tr.w}$ and $\sum M_{tr.s}$ are total transformed mass in water and sediments, respectively.
 959 $\sum M_{ads}$ and $\sum M_{des}$ are the total adsorbed and desorbed mass, respectively. Err (%) is the mass balance error of
 960 each simulation.
 961

Pesticides	2014-2015								
	Influx/Outflux		Total mass		Transformation		Adsorption-Desorption		MBE
	$\sum M_{in}$	$\sum M_{out}$	M_w	M_s	$\sum M_{tr.w}$	$\sum M_{tr.s}$	$\sum M_{ads}$	$\sum M_{des}$	Err (%)
Bentazon	51.51	38.55	0.11	3.48	8.95	1.06	8.56	4.02	1.25
Boscalid	5.42	3.40	0.00	1.97	0.00	0.17	2.14	0.00	2.21
Chlorotoluron	8.94	6.11	0.00	2.40	0.08	0.36	2.76	0.00	0.00
Diflufenican	4.23	2.69	0.00	1.23	0.01	0.31	1.53	0.00	0.00
Mesotrione	-	-	-	-	-	-	-	-	-
S-metolachlor	13.73	9.74	0.02	0.48	3.27	0.21	1.00	0.31	0.01
Quinmerac	46.98	33.78	0.29	8.02	5.07	1.05	22.69	13.62	2.63
Mean	21.80	15.71	0.07	2.93	2.90	0.53	6.45	2.99	1.02

962

Pesticides	2016-2017								
	Influx/Outflux		Total mass		Transformation		Adsorption-Desorption		MBE
	$\sum M_{in}$	$\sum M_{out}$	M_w	M_s	$\sum M_{tr.w}$	$\sum M_{tr.s}$	$\sum M_{ads}$	$\sum M_{des}$	Err (%)
Bentazon	14.42	11.52	0.00	0.18	2.11	0.60	2.33	1.55	0.00
Boscalid	5.10	3.48	0.01	1.45	0.00	0.16	1.61	0.00	0.01
Chlorotoluron	-	-	-	-	-	-	-	-	-
Diflufenican	-	-	-	-	-	-	-	-	-
Mesotrione	-	-	-	-	-	-	-	-	-
S-metolachlor	10.02	6.28	0.01	0.06	3.40	0.26	0.48	0.17	0.01
Quinmerac	-	-	-	-	-	-	-	-	-
Mean	9.85	7.10	0.01	0.56	1.84	0.34	1.47	0.57	0.01

963

Pesticides	2017-2018								
	Influx/Outflux		Total mass		Transformation		Adsorption-Desorption		MBE
	$\sum M_{in}$	$\sum M_{out}$	M_w	M_s	$\sum M_{tr.w}$	$\sum M_{tr.s}$	$\sum M_{ads}$	$\sum M_{des}$	Err (%)
Bentazon	-	-	-	-	-	-	-	-	-
Boscalid	-	-	-	-	-	-	-	-	-
Chlorotoluron	-	-	-	-	-	-	-	-	-
Diflufenican	1.65	0.06	1.59	8.95	6.83	0.47	0.01	0.46	2.06
Mesotrione	13.52	5.36	8.15	49.52	25.64	10.35	3.11	7.25	18.65
S-metolachlor	53.88	45.97	7.92	295.85	190.05	51.91	51.30	0.61	9.11
Quinmerac	5.86	1.96	3.90	26.19	17.86	2.47	2.16	0.31	8.09
Mean	-	-	-	-	-	-	-	-	-

964

Pesticides	2018-2019								
	Influx/Outflux		Total mass		Transformation		Adsorption-Desorption		MBE
	$\sum M_{in}$	$\sum M_{out}$	M_w	M_s	$\sum M_{tr.w}$	$\sum M_{tr.s}$	$\sum M_{ads}$	$\sum M_{des}$	Err (%)
Bentazon	0.64	0.01	0.63	25.64	23.02	1.98	1.66	0.33	2.24
Boscalid	-	-	-	-	-	-	-	-	-
Chlorotoluron	-	-	-	-	-	-	-	-	-
Diflufenican	-	-	-	-	-	-	-	-	-
Mesotrione	0.32	0.02	0.29	68.18	49.84	18.02	2.67	15.35	26.17
S-metolachlor	-	-	-	-	-	-	-	-	-
Quinmerac	14.97	0.47	14.50	123.35	97.95	10.42	8.24	2.18	35.31
Mean	0.64	0.01	0.63	25.64	23.02	1.98	1.66	0.33	2.24

Pesticides	2019-2020								
	Influx/Outflux		Total mass		Transformation		Adsorption-Desorption		MBE
	$\sum M_{in}$	$\sum M_{out}$	M_w	M_s	$\sum M_{tr.w}$	$\sum M_{tr.s}$	$\sum M_{ads}$	$\sum M_{des}$	Err (%)
Bentazon	3.16	2.11	0.09	0.39	0.54	0.03	0.54	0.12	0.00
Boscalid	-	-	-	-	-	-	-	-	-
Chlorotoluron	12.80	11.20	0.00	1.36	0.04	0.20	1.56	0.00	0.00
Diflufenican	8.24	6.10	0.01	1.80	0.01	0.32	2.12	0.00	0.00
Mesotrione	-	-	-	-	-	-	-	-	-
S-metolachlor	20.74	13.32	0.88	1.45	4.96	0.14	1.80	0.21	0.00
Quinmerac	-	-	-	-	-	-	-	-	-
Mean	11.24	8.18	0.24	1.25	1.39	0.17	1.50	0.08	0.00

968 **Table A.6:** The mean percentage (%) of each process to the total intercepted/INPUT mass of pesticides.

	Photolysis	Biotransformation in water	Biotransformation in sediments	Adsorption	Desorption
Bentazon	8.68	5.21	2.14	14.63	6.82
Boscalid	0.00	0.04	3.18	35.49	0.00
Chlorotoluron	0.35	0.24	2.82	21.53	0.00
Diflufenican	0.09	0.06	5.45	28.27	0.00
Mesotrione	0.27	4.52	17.86	36.19	10.68
S-metolachlor	0.25	23.97	1.25	5.87	1.26
Quinmerac	0.46	7.94	1.70	35.26	19.32

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972 **6.8 Extrapolation: Efficiency abacus**973 **Table A.7:** The mean efficiency (%) of the Rampillon AP according to different pond areas. A is the real AP
974 area (5270 m²).975 **Surface area = A**

	2014-2015	2016-2017	2017-2018	2018-2019	2019-2020
Bentazon	26.58	47.24	-	26.33	46.52
Chlorotoluron	29.27	-	-	-	12.52
Diflufenican	34.89	-	27.77	-	42.44
Mesotrione	-	-	48.97	52.54	-
S-metolachlor	31.42	75.19	36.59	-	50.17
Quinmerac	30.40	-	33.17	44.71	-

976

977 **Surface area = A+10 000 m²**

	2014-2015	2016-2017	2017-2018	2018-2019	2019-2020
Bentazon	50.06	71.32	-	49.49	68.90
Chlorotoluron	54.70	-	-	-	52.96
Diflufenican	60.73	-	51.86	-	67.24
Mesotrione	-	-	72.80	77.01	-
S-metolachlor	56.05	90.02	62.74	-	
Quinmerac	53.92	-	55.35	71.53	-

978

979 **Surface area = A+20 000 m²**

	2014-2015	2016-2017	2017-2018	2018-2019	2019-2020
Bentazon	61.50	80.26	-	61.47	77.84
Chlorotoluron	66.64	-	-	-	64.97
Diflufenican	71.87	-	63.81	-	76.99
Mesotrione	-	-	81.46	84.88	-
S-metolachlor	67.13	93.75	73.65	-	79.43
Quinmerac	64.13	-	65.78	80.92	-

980

981 **Surface area = A+30 000 m²**

	2014-2015	2016-2017	2017-2018	2018-2019	2019-2020
Bentazon	68.35	84.95	-	68.85	82.77
Chlorotoluron	73.58	-	-	-	72.09
Diflufenican	78.07	-	70.99	-	82.25
Mesotrione	-	-	85.94	88.74	-
S-metolachlor	73.56	95.45	79.60	-	83.75
Quinmerac	69.92	-	72.11	85.67	-

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986 **Surface area = A+40 000 m²**

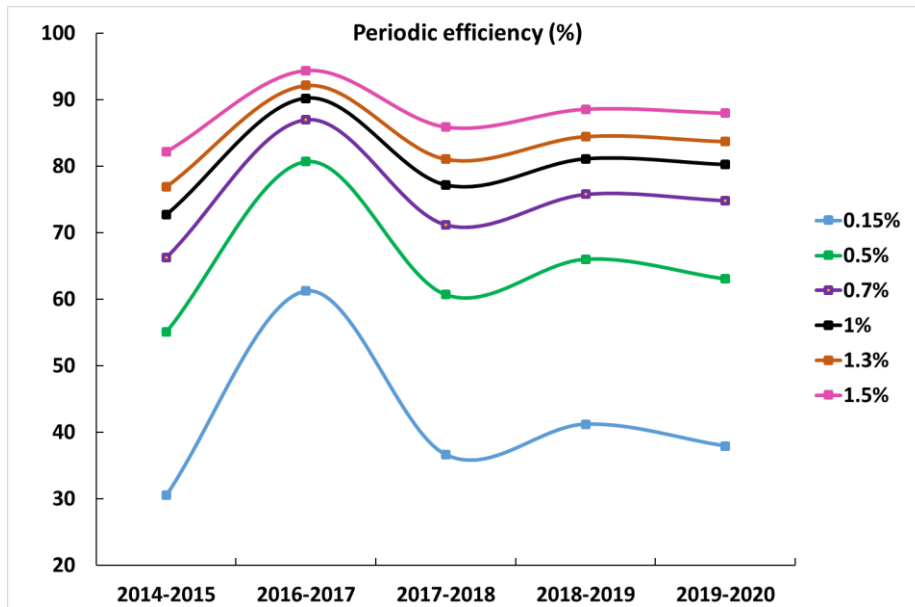
	2014-2015	2016-2017	2017-2018	2018-2019	2019-2020
Bentazon	72.95	87.83	-	73.85	85.89
Chlorotoluron	78.12	-	-	-	76.81
Diflufenican	82.03	-	75.80	-	85.54
Mesotrione	-	-	88.68	91.03	-
S-metolachlor	77.82	96.43	83.35	-	86.54
Quinmerac	73.67	-	76.42	88.53	-

987

988 **Surface area = A+50 000 m²**

	2014-2015	2016-2017	2017-2018	2018-2019	2019-2020
Bentazon	78.76	91.20	-	80.21	89.65
Chlorotoluron	83.71	-	-	-	82.68
Diflufenican	86.80	-	81.82	-	89.45
Mesotrione	-	-	91.85	93.62	-
S-metolachlor	83.16	97.50	87.81	-	89.95
Quinmerac	78.27	-	81.95	91.80	-

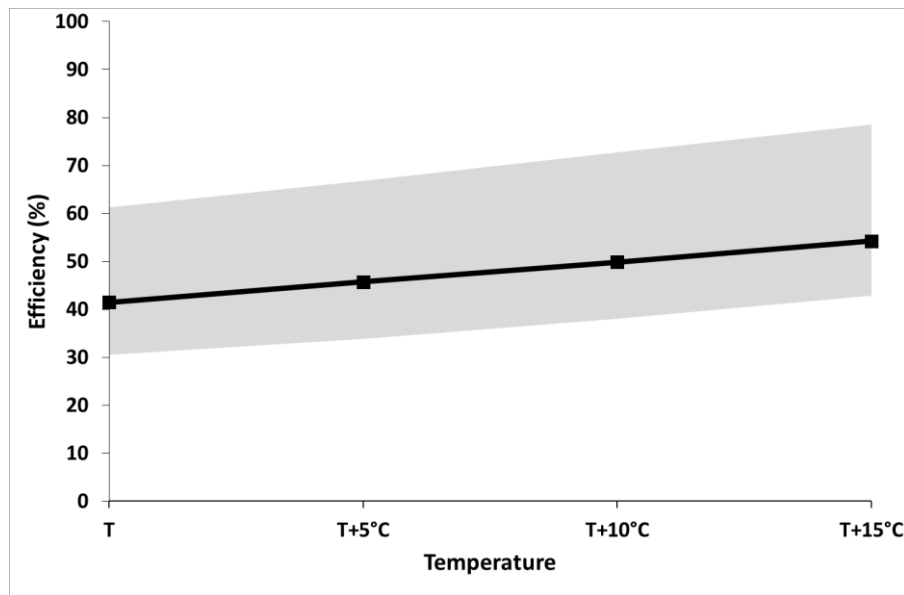
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991 **Figure A.8:** The annual efficiency of the Rampillon AP to dissipate pesticides from the inlet to the outlet according
 992 to different sizes of the pond. The x-axis represents the evaluated periods and each color refers to the percentage
 993 (%) of the area occupied by the AP in the total catchment area (355ha). The actual AP area is 0.15% (5270 m²).

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995

996 **Figure A.9:** The mean efficiency of the Rampillon AP to dissipate pesticides from the inlet to the outlet according
 997 to increasing temperatures. T refers to the actual daily temperature in the Rampillon AP. The upper and lower grey
 998 areas refer to the discrepancy between the mean and the maximum and minimum efficiencies, respectively.

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Table A.8: Summary of pesticides monitoring data. The selected periods correspond to monitoring data without artifacts. In addition, the pesticide re-mobilization periods were not considered (i.e., pesticide outlet concentration $C_{out} >$ inlet concentration C_{in}). Days refers to the total duration of each period. $Q_{in,max}$ ($\mu\text{g.L}^{-1}$) is the maximum water flow rate intercepted by the Rampillon AP. $Q_{in,mean}$ ($\mu\text{g.L}^{-1}$) is the mean water flow rate intercepted by the Rampillon AP during the corresponding period. C_{max} ($\mu\text{g.L}^{-1}$) is the maximum detected concentration of each pesticide, C_{mean} ($\mu\text{g.L}^{-1}$) is the mean detected concentration during the corresponding period, and the DR is the detection frequency of pesticides. T ($^{\circ}\text{C}$) and HRT (d) are the average temperature and hydraulic residence time of each period, respectively. TUR (FTU) is the mean turbidity, NO_3^- (mg.L^{-1}) is the mean nitrate concentration, TOC (mg.L^{-1}) is the mean total organic carbon concentration, and DOC (mg.L^{-1}) is the mean total dissolved organic carbon concentration. Each pesticide is associated with its type: (H) Herbicides, (F) Fungicides.

Period	Duration (days)	$Q_{in,max}$ (L.s^{-1})	$Q_{in,mean}$ (L.s^{-1})	Study case	Pesticide	C_{max} ($\mu\text{g.L}^{-1}$)	C_{mean} ($\mu\text{g.L}^{-1}$)	Detection frequency	T	HRT	TUR	NO_3	TOC	DOC
14/10/2014 - 03/06/2015	233	87.44	19.45	1	Bentazon (H)	0.443	0.099	100%	8.0 5	8	8.88	10.8 7	7.53	4.03
				2	Boscalid (F)	0.064	0.029	33.30%						
				3	Chlorotoluron (H)	0.074	0.049	18.20%						
				4	Diflufenican (H)	0.026	0.01	54.50%						
				5	S-Metolachlor (H)	0.22	0.033	87.90%						
				6	Quinmerac (H)	0.921	0.238	51.50%						
07/11/2016 - 12/09/2017	310	24.2	0.73	7	Bentazon (H)	0.263	0.1106	96.80%	11. 2	14	7.98	10.6 8	6.95	4.21
				8	Boscalid (F)	0.079	0.0387	35.50%						
				9	S-Metolachlor (H)	12	1.959	19.40%						
12/09/2017 - 13/06/2018	275	147.61	27.63	10	Diflufenican (H)	0.047	0.015	58.30%	9.2	7	20.4 1	10.5 7	23.3 3	13.0 7
				11	Mesotrione (H)	1.096	0.5665	16.70%						
				12	S-Metolachlor (H)	8	0.5836	91.70%						
				13	Quinmerac (H)	0.331	0.0897	44.40%						

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1007 **Table A.8** (continued)

Period	Duration (days)	Qinmax (L.s ⁻¹)	Qinmean (L.s ⁻¹)	Study case	Pesticide	Cmax (µg.L ⁻¹)	Cmean (µg.L ⁻¹)	Detection frequency	T	HRT	TUR	NO3	TOC	DOC
17/10/2018 - 03/07/2019	260	72.32	9.95	14	Mesotrione (H)	1.449	0.5527	22.20%	8.63	9	16.8	13.2	33	20.7
				15	S-Metolachlor (H)	0.4	0.1039	44.40%						
				16	Quinmerac (H)	2.681	0.758	25.90%						
30/10/2019 - 19/05/2020	203	91.42	16.23	17	Bentazon (H)	0.082	0.0497	21.40%	8.45	6	7.1	10.2	6.4	3.7
				18	Chlorotoluron (H)	0.113	0.0757	42.90%						
				19	Diflufenican (H)	0.039	0.017	78.60%						
				20	S-Metolachlor (H)	0.77	0.0767	92.90%						

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