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# 1 A lumped model to simulate nitrate concentration 2 evolution in groundwater at catchment scale

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9

## 10 Summary

11 Groundwater nitrate contamination requires implementation of measures to reduce the impact of  
12 agricultural sources. Models appear as a way to understand the nitrate transfer and its temporal  
13 trend as well as a forecasting tool useful for decision making. Given their ease of implementation  
14 compared to discretized models, lumped models seem appropriate tool for stakeholder purposes  
15 but remain rarely used in transport modelling. The lumped model BICHE, simulating both  
16 hydrologic and nitrate transport in a coupled way, was applied on three sites having contrasted  
17 hydrogeological characteristics and under various agricultural pressures. The model has an  
18 automatic calibration procedure which is used under constraints fixed by the operator. It was  
19 executed on three catchments on a long duration simulation (about 30 years) and performed  
20 again 5 years later. This extension of the dataset allowed to evaluate the robustness of the  
21 calibration. Whether for the water level or the nitrate concentrations modelling, the performance  
22 of the model was almost not altered, confirming the validity of the calibration. Results highlighted  
23 model performance for long-term trend of nitrate concentration whereas very short-term  
24 variations were less well reproduced, especially for the studied site showing large weekly  
25 fluctuations. Certain data, in particular agricultural data, are particularly difficult to obtain for the  
26 whole catchment at a detailed time step and the use of rough estimation for these data generate

27 uncertainties. This aspect is however not prohibitive since the purpose of such modelling is to  
28 forecast global trends in nitrate concentrations under various types of scenarios. This modelling  
29 for the three sites allowed an analysis of the effect of agricultural changes in term of nitrate  
30 concentration but also on time lag between the implementation of these changes and their  
31 impact on groundwater quality. Considering the ease of implementation, the robustness of model  
32 and the quality of the simulations obtained, we confirm that this tool is particularly relevant for  
33 stakeholders to address groundwater nitrate contamination.

34

## 35 Keywords

36 Groundwater quality; Lumped model; Nitrate; Agricultural programs of measures, Impact; Lag  
37 time

38

## 39 1 Introduction

40 In Europe, the Nitrate Directive (91/676/EEC), adopted in 1991, concerns the protection of  
41 surface and ground waters against nitrate contamination by preventing nitrate from agricultural  
42 sources and by promoting the use of good farming practices. This directive is closely relative to  
43 the European water framework directive (2000/60/EC), which aims to achieve the objective of  
44 good chemical status by defining and implementing the necessary measures and to the  
45 groundwater directive (2006/118/EC) which confirms the 50 mg/l quality standard as an  
46 European standard for nitrate concentration in groundwater.

47 The implementation of the measures can be difficult to accept by local actors, especially if we  
48 lack concrete elements to quantify the expected impact of these measures. This is especially  
49 true for groundwater where the time lag between the change of agricultural practices and the

50 impact on groundwater quality can be several years or even decades (Donald, et al., 2010;  
51 Gutierrez and Baran, 2009).

52 Thus, the use of models appears as an alternative to the *a priori* evaluation of the effects of  
53 measures.

54 Dynamic, process-based catchment models are designed to represent the processes governing  
55 catchment hydrology and water quality, and may therefore be useful tools for catchment  
56 management. But, the complexity of these types of models brings a number of issues related to  
57 parameter uncertainty (Jackson-Blake, et al., 2017) and parameterization (Woodward, et al.,  
58 2017; Knowling, et al., 2019). To produce reliable predictions, these models require large  
59 quantities of detailed data to characterize the physical properties of the model domain and  
60 parameters (Hong, et al., 2017). These issues are generally due to low information from  
61 geological and hydrological data combined with the complexity and uncertainty of representing  
62 the subsurface processes (Woodward, et al., 2016). Despite their complexity, their performance  
63 could be poor (Refsgaard and Hansen , 2010). If the use of complex model might be useful in  
64 terms of knowledge of the processes, it has limitations when applied in an operational context  
65 (Perrin, et al., 2001). Besides, it was demonstrated that very simple models can achieve a level  
66 of performance almost as high as models with more parameters (Perrin, et al., 2001).

67 So, simpler approaches are needed for decision making based on readily available data  
68 (Jackson-Blake, et al., 2017). As a consequence, there is a renewed interest for lumped  
69 conceptual models (Woodward, et al., 2017 ; Charizopoulos, et al., 2017). Some previous works  
70 have already shown the effectiveness of lumped model to provide a simple approach to the  
71 simulation of groundwater nitrate concentrations that requires little data (Hong, et al., 2017).  
72 Nevertheless, codes and applications to different case studies remain scarce.

73 BICHE (Bilan CHimique des Eaux – Water chemistry balance), developed by BRGM (Thiéry and  
74 Seguin, 1985), is a lumped model, which simulates nitrate transfer together with the hydrological  
75 functioning at the scale of a catchment. The model has a conceptual structure represented by a

76 cascade of linear tanks interacting through mathematical functions to describe the fluxes (water  
77 or nitrate) between the tanks. BICHE considers the catchment as an undivided entity and uses  
78 lumped values of input variables and parameters. Crop diversity is taken into account but not its  
79 location within the catchment. Therefore, input variables need to be aggregated and measured  
80 parameters are not representative of the whole. As lumped parameters cannot be measured on  
81 the field, such parameters can only be determined by trial-and-error calibration within physical  
82 bounds. Moreover, as several combination of physical parameters may produce the same  
83 simulation, semi-empirical parameters, such as recession constants, are used. Although, the  
84 model does not take into account plot location within a catchment, it becomes particularly useful  
85 when using prospective scenarios or comparison of different scenarios. In the model, nitrate  
86 concentration which depends on the fertilizer applications, consumption by crops and soil  
87 interaction is transferred towards surface or groundwater according to characteristic of the  
88 catchment and climatic conditions (Thiéry, 1988; Thiéry, and Seguin., 1988). Parameters are  
89 calibrated automatically using optimization routines. This calibration process seek the best fit of  
90 simulated data to measured time series (observed groundwater levels and nitrate  
91 concentrations). This methodology is classical with lumped model and is improved when  
92 optimization is framed and constrained by expert evaluation (Gharari, et al., 2015). The  
93 possibility is given to separate the calibration process in two phases: first establish the  
94 hydrological fitting and then calibrate the nitrate transfer. This may be useful in the first stage of  
95 calibration.

96 Thanks to a relatively limited number of parameters, automatic calibration, and a low  
97 computation time, the application of the BICHE model is relatively easy and straightforward. This  
98 reinforces its operational purpose. However the strengths and limitations of this tool should be  
99 well understood prior to its use beyond research projects.

100 Thus, the main objective of this paper is to demonstrate that BICHE is a tool for stakeholders  
101 and decision makers to set up or assess agricultural and environmental programs of measures.

102 To achieve this objective, we carried out a three-folded evaluation of the model's potential. The  
103 first step of this evaluation was to assess the ability of the lumped model BICHE to simulate the  
104 observed time series nitrate concentrations in groundwater for various hydrogeological and  
105 agricultural contexts over long time periods (minimum 10 years). The second step was to  
106 evaluate the robustness of the calibration by using/simulating an extended set of data (i.e by  
107 simulating additional years using the initial calibration). The last step was to assess model  
108 interest for decision makers thanks to a retrospective analysis of the implemented agricultural  
109 measures (i.e by simulating an alternative set of input data considering continuity of practices as  
110 they were before the initiation of environmental measures).

111 The dataset for this evaluation is composed of groundwater level and nitrate concentration time  
112 series on three agricultural catchments, where surveys of agricultural practices were available  
113 over a long period. To better highlight the ability of the model to simulate water and nitrate  
114 transfers in different hydrogeological and agronomic contexts, the three catchments have been  
115 selected to serve as representative combinations of some aquifers, soils and climate of France  
116 and Western Europe.

## 117 2 Materials and methods

### 118 2.1.1 Model description

119 The chemical transfer model BICHE is derived from the lumped hydrologic tank model Gardenia  
120 (Thiéry, 1988, Thiéry, 2015). The hydrological model is a tank model that simulates the water  
121 cycle from the rain falling on the basin to the outlet discharge (a river, a spring or a pumping  
122 borehole). The input data are the atmospheric precipitation (rainfall and snow) on the catchment  
123 area and the potential evapotranspiration (PET) and when necessary water pumping for  
124 irrigation. A calibration is done on a series of discharges at the basin outlet or of groundwater  
125 levels at one spot, or both. On the studied sites which are exclusively groundwater catchments,  
126 the calibration only used groundwater fluctuations. The water cycle is represented by a system

127 of three compartments (tanks): 1) the first one considers water exchanges between soil and  
128 atmosphere (precipitation and evapotranspiration by computing at each time step a water  
129 balance generating actual evapotranspiration and “effective rainfall”, 2) an intermediate tank  
130 simulates rapid flow towards the outlet river and groundwater recharge. This rapid flow stands  
131 for runoff or karst flow which generates a rapid impact on water flow, and 3) the third one  
132 simulates slow flow representing slow groundwater motion and contribution to the observed  
133 system (river or water table). Flow between the three tanks are governed by a maximum of six  
134 hydrological parameters described in appendix A.

135 Nitrate transfer is based on the same structure as water transfer: a nitrate content is associated  
136 to each flow in each compartment so that the computed mass fluxes at the output of the system  
137 allows the comparison of simulated and observed nitrate concentration (Fig. 1) at the outlet of  
138 the basin. To compute nitrate content in the first compartment, one must input into the model the  
139 time evolution of four series over the simulation duration (and even starting before for model  
140 initialization): 1) the nitrogen spread as fertilizer over the catchment area during the growing  
141 season; 2) crop nitrogen needs during the various seasons; 3) natural soil mineralization; and 4)  
142 the crop nitrogen residual mineralization after harvest.

143 The model computes at a chosen time step (from hourly to yearly, but usually monthly for nitrate  
144 computation on the long run), the balance between the quantities of nitrogen which are added  
145 (by fertilizers) or transformed (by mineralization), withdrawn by the plants or which flows out of  
146 the soil compartment. Exchanges with immobile water or adsorption effects are taken into  
147 account through exchange coefficients thus simulating retardation effects. The complete list and  
148 description of parameters is given in Appendix A.

149 Calibration consists in comparing observed values with simulated data. The model has an  
150 automatic calibration process based on a non-linear optimization algorithm adapted from the  
151 Rosenbrock method (Rosenbrock, 1960). Calibration is done in a semi-automatic way: the user  
152 provides an initial value and a range of variation for each parameter, to keep the parameters

153 within plausible values and ensure that secondary results (as recharge computation) remain  
154 consistent. The user may also fix values of parameters he knows best, thus reducing the number  
155 of optimized parameters. Previous work showed that imposing constraints prevents lumped  
156 model from overfitting during calibration and improve reliability outside the calibration period  
157 (Gharari, et al., 2015). As hydrological parameters have an influence on mass transfer, but mass  
158 transfer parameters have no influence on water flows, we chose to first calibrate the hydrologic  
159 parameters in order to reproduce the water table level fluctuations at one observation well, and  
160 then, the mass transfer parameters to simulate the nitrate content in the outflow (or in the  
161 aquifer). Alternatively, the hydrological parameters and the mass transfer parameters can be  
162 calibrated simultaneously. This sometimes leads to better fitting albeit less controlled  
163 parametrization justifying our choice to proceed in two steps.

164 The water level fluctuation and the concentration level in the aquifer at the beginning of the  
165 simulation depend on historical data that is usually unknown. This problem is solved by using a  
166 “warm-up period” to initialize the model. In our simulations, the warming-up process consisted in  
167 starting the simulation a long period before the beginning of the water levels and concentration  
168 monitoring, repeating existing known input series.

169 The calibration process is based on maximizing the Nash criterion (Nash and Sutcliffe, 1970)  
170 between the observed and simulated series. An overall goodness of fit criterion, “F”, combines  
171 the Nash criterion of each simulation (groundwater level and nitrate content) (appendix A). Its  
172 maximal possible value for a perfect fit is 1.

173 A potential disadvantage of automatic calibration based on typical objective functions is that they  
174 do not account for temporal offsets between predicted values and observed data. A timing  
175 difference of several days does not imply a bad fit when the modelling period encompasses  
176 several years, but can have a major effect on the goodness of fit criterion. To minimize this  
177 limitation, in addition to the evaluation using the goodness of fit criterion, the visual agreement



178 between the curve of simulated chronicle and observed chronicle was also given consideration  
179 in the calibration process.

180

## 181 2.2 Studied catchments

182 The three studied groundwater catchments were selected because they presented three  
183 different hydrogeological, climatic and agricultural contexts (Table 1). Their sizes varied from 4  
184 to 50 sq. km.

185 The studied aquifers correspond to basement formations, karstified limestone and fissured  
186 limestone (Fig. 2). The low water period generally occurs in November, September and August,  
187 respectively. Groundwater levels have intra-annual fluctuations of less than 1m (limestone site)  
188 to around 8 m (karstic site). Based on the water level series, the basement, karstic and  
189 limestone sites can be described as not very reactive, very reactive or mixed, respectively.

190 The mean rainfall and the mean potential evapotranspiration are slightly contrasted: rainfall is  
191 highest in the basement site (766 mm/yr) and lowest in the limestone site (699 mm/yr) and  
192 Potential Evapotranspiration varies according to the sites between 688 mm/yr (basement site)  
193 and 846 mm/yr (karstic site).

194 The three sites, located in agricultural contexts, exhibit different initial agricultural pressure and  
195 different temporal evolution. Indeed, for each of the sites, in response to the increase of water  
196 resource contamination by nitrate in the last 30 to 50 years, the stakeholders have implemented  
197 different measures i.e. both regulatory measures linked, for example to the Nitrate Directive and  
198 applied throughout the territory and more local measures. For the basement site, their strategy  
199 was based on land use modification, initiated in 1995, resulting in a replacement of vegetables  
200 by meadow (the surface in meadow rose from 1% in 1995 to 43% in 2013 of the total utilized  
201 agricultural area). For the karstified limestone, land use has a significant proportion of straw  
202 cereals (wheat, barley). Noticeably rapeseed surfaces have increased the most over the period  
203 studied to the detriment of grass. The Agricultural Chamber led the major action of management

204 by providing a very close agronomic advices from 2003-2004 onwards on around 80% of the  
205 cultivated surfaces. For the limestone site, land use shows that straw cereals (in rotation with  
206 rapeseed) are by far the most important crops. Grass surfaces have decreased, while rapeseed  
207 areas are increasingly from the 1990's. The first action plan on this catchment start in 1991  
208 leading to the conversion of about 1% of the cultivated surface into poplars plantation. From  
209 2003-2004 onwards, 80% of the plots of the catchment are monitored; advices were provided to  
210 the farmers to improve fertilization by the agricultural chamber.

### 211 2.3 Existing and estimated input data

212 Monthly rainfall and evapotranspiration, available during the whole duration of the simulation at  
213 three meteorological stations of Météo-France (national meteorological and climate operator)  
214 close to the studied sites were used. Water level time-series are available for 11, 21 and 23  
215 years while nitrate concentrations time-series are available for 31, 41 and 35 years in the  
216 basement, karstic and limestone sites, respectively.

217 Land uses and practices are known for several years thanks to detailed interviews of farmers.  
218 For the basement site, surveys were performed between 1991 and 1995, and between 2008 and  
219 2013. For the karstic site, data were collect between 1992 and 2009. For the limestone site,  
220 surveys were performed in 1991, 1999 and between 2007 and 2015. Others sources of  
221 information were used to fill the gaps. The Ministry of Agriculture feed a national database since  
222 1970 with data (Utilized Agricultural Area - UAA and distribution of this area between crops) at  
223 communal scale. The statistics are available for five dates 1970, 1979, 1988, 2000 and 2010.  
224 For years after 2010 i.e. for the period 2011-2015, surface occupations were collected at the plot  
225 scale using a geographical information system application (recently developed and used as a  
226 reference for the instruction of aid of the common agricultural policy in France) (Agreste, 2018).  
227 Extrapolation (to extend the data set) or interpolation between input data were used when no  
228 value were available.

229 The model has four input series representing crop management: 1) Fertilization 2) Crop nitrogen  
230 need 3) Soil mineralization 4) Crop residue mineralization.

231 The N consumption of each crop was computed using nitrogen theoretical absorption curves  
232 (e.g. Justes, et al., 1994 for wheat). Then, nitrogen absorption curves were adjusted according  
233 to the local crop yield data when available or departmental yield data otherwise. Local data were  
234 available between 2001 and 2009 for karstic site and between 2007 and 2015 for limestone site.  
235 Departmental yields were available from 1989 to present. Those data are available on a French  
236 Agriculture Ministry database (Agreste, 2018). The N fertilization for each crop was computed  
237 using the N balance model proposed by COMIFER (COMIFER, 2013) for France and  
238 parameters were modified according to the local survey. In each catchment, data from the  
239 agricultural chamber were available to adjust the doses at different crop growth stages.

240 The mineralization of soil was computed from soil organic matter with an adapted equation from  
241 the LIXIM model (Mary, et al., 1999). The adaptation consists to use only one pool of nitrogen,  
242 and some improvements to calculate the rate of degradation (Valé, 2006). The crop residuals  
243 mineralization was calculated by using flat-rate value for each crop (COMIFER, 2013).

244 For each model time step, the value of fertilization, N consumption, mineralization and crop  
245 residue mineralization of one specific crop is multiplied by its surface to represent the relative  
246 value. The relative values of each crop are summed up to represent the fertilization, N  
247 consumption, mineralization and crop residue mineralization for the whole catchment. The input  
248 files were compiled by weighting the influence of each crop according to its surface in the  
249 catchment, for each year.

## 250 2.4 Three-folded evaluation of the model potential

### 251 2.4.1 "Assessment of the model performances"

252 A first dataset ending in 2010 was prepared for each selected catchment. The starting date for  
253 the different simulations is dependent on the first available nitrate concentration record in each

254 selected basin i.e., 1985 for the basement site, 1975 for the karstic site and 1988 for the  
255 limestone one. The simulations used a monthly time step.

#### 256 2.4.2 “Assessment of the model robustness”

257 The second step aimed to assess the robustness of the model by extending the initial data set  
258 for five years (input data and observed data). For this second set of simulations, the previously  
259 used data was completed by series of new data (between 2011 and 2015), acquired and  
260 collected with the same methodology. This second set of simulation was performed in a second  
261 phase of the project that was executed five year after the first one. The simulation was  
262 performed without any new calibration procedure. The aim is to assess whether the quality of the  
263 simulation without recalibration is acceptable or not or whether a new calibration is necessary.

#### 264 2.4.3 “Assessment of the interest of the model retrospective approach”

265 The last step was set up as a demonstrative use of BICHE by decision makers in an evaluation  
266 of an environmental and agricultural policy. A retrospective analysis was performed to evaluate  
267 the impact of the implemented measures several years ago by comparing simulations with and  
268 without this specific action. This last step is only possible if the two former ones have proved  
269 valuable. Then, considering that the model correctly simulates and predict reality, the  
270 retrospective analysis is a “what if” situation where events are assumed not to have happened  
271 and measures not to have been taken. A theoretical scenario “no agro-environmental measure”,  
272 was built, irrespective of the national and local measures implementation, by considering that the  
273 land use and farming practices observed before the 1991 (i.e. date of Nitrate directive  
274 implementation) were still in practice in 2015, i.e. by repeating the 1989/1990 agronomic data  
275 from 1990 to 2015. On two of the sites, the local measures having been implemented  
276 immediately after the application of the Nitrate Directive, this scenario starting date makes it  
277 possible to evaluate the cumulative effect of the two types of measures.

278

## 279 2.5 Results and discussion

### 280 2.5.1 “Assessment of the model performances”

281 For the 3 studied sites, the goodness of fit criteria (the Nash criteria, see appendix A) are  
282 satisfactory (Moriasi et al, 2015) whatever the type of agronomic and hydrogeological situations.  
283 The Nash criteria are satisfactory for the hydrological modelling (values of 0.76, 0.71 and 0.50  
284 for the basement, karstic and limestone sites respectively- Fig. 3a, 4a, 5a) because the  
285 simulations match seasonal fluctuations as well as interannual variations. The Nash criterion is  
286 lower for nitrate simulations in the karstic (0.61- Fig. 4b) and limestone (0.50- Fig. 5b) sites  
287 where concentration variation (which can be up to 10 mg/L between two adjacent measurements  
288 in the karstic site and even 20 mg/L in the limestone site) cannot be reproduced. For this last  
289 site, the Nash criterion computed on the average of the 12 consecutive measurements increases  
290 from 0.50 to 0.75. In the basement site which shows no short-term fluctuation and seems to  
291 have much more inertia, the concentration simulated has a better Nash criterion (0.94- Fig. 3b).  
292 For all sites a visual inspection of the graphs shows that the simulations reproduce correctly the  
293 smoothed concentration evolutions. These results highlight the good performance of BICHE as a  
294 lumped model in the simulation of groundwater level and nitrate concentration. Groundwater  
295 level are better calibrated than nitrate concentrations except when the aquifer system provides  
296 considerable damping of the input signal, to the point of masking its short-term temporal  
297 variability and only retaining its trend. This situation is however less common. Previous work has  
298 already shown that simple models can simulate hydrological phenomena (Orth, et al., 2015), but  
299 that phenomena related to water quality may require additional complexity (Medici, et al., 2012).  
300 It may seem paradoxical, but the quality of the calibration may not be well translated by the Nash  
301 criterion. As discussed above, the Nash criterion is very dependent on the smoothness of the  
302 input data, which tend to better illustrate the trends of the series. In a noisy dataset, the Nash  
303 criterion is lower but the trend can be properly simulated just as well or even better. Pluri-annual

304 trends are indeed what matters in such simulations, aiming at orientating policies rather than  
305 looking for the detailed evolution of concentration in the aquifer.

306 If reaching a better goodness of fit for nitrate concentration can be obtained with a more complex  
307 model, it is however not in line with a need for simplification, guided by the following reasons.

308 The increase in the number of parameters may improve the calibration but over parametrization  
309 also result in increasing the number of equivalent solutions. Refining the time step (e.g. from  
310 monthly to daily) may increase short time variability, but the accuracy and quality of data input is  
311 not fine enough to be used at such a scale. For instance, it is impossible to know the exact date  
312 of fertilization when no record was taken. Additionally, many aquifer systems, as the karstic and  
313 limestone sites of this study, show variable vertical transfer velocities resulting in erratic  
314 variations of the observed concentration. At the end, the objective being to support decision  
315 making in environmental management, the goal of the model should be to promote simulation of  
316 major trends in nitrate concentration rather than to focus on unnecessary details which have no  
317 impact on the input – output relationship and the predictive capabilities of the model (Kirchner,  
318 2006; Siebert, 2003). Therefore, the tested lumped model is assumed to be highly valuable for  
319 stakeholders and decision makers as it is a relatively simple, computationally efficient method for  
320 predicting nitrate time-series concentration in groundwater in contrasted hydrogeological and  
321 agricultural contexts.

#### 322 2.5.2 Assessing the model robustness

323 The purpose of this second series of simulations is to evaluate whether the model behaves like  
324 the real soil and aquifer system not only within the calibration period but also in prediction, that  
325 is, when no observed value can sustain the calibration process. Running the model with the  
326 extended set of five years (2011-2015) without any new calibration process (keeping the exact  
327 parameters of the simulations presented in 3.1.1), it will show its robustness and ability to be  
328 used in predictive mode.

329 For the 3 studied sites, for both water level (Fig. 3a, 4a, 5a) and nitrate concentration (Fig. 3b,  
330 4b, 5b), the values simulated between 2011 and 2015 by using the parameters calibrated with  
331 shorter series are consistent with the observed values. The Nash criterion of hydrological  
332 simulations is still satisfactory (Moriasi et al, 2015) and even improved in the three sites (0.79,  
333 0.79, 0.53 for basement, karstic and limestone site respectively). The five years are not  
334 exceptional ones on the climatic point of view and correspond to the normal years already  
335 simulated. Since the calibration reproduce these normal years correctly (as opposed to  
336 exceptional years), the extension of the data improves the adjustment criterion.

337 The matching of the nitrate concentration simulations is slightly degraded by the extension of  
338 data. However the Nash criterion remain satisfactory (0.90, 0.56, 0.44 for basement, karstic and  
339 limestone site respectively). Paradoxically, it is on the basement site, where the fit criterion is  
340 higher and its decrease is the smallest, that the fit seems the most degraded visually. This visual  
341 effect is linked to the smoothness of the observed time series, from which any small deviation is  
342 easily spotted. The discrepancy is however less than 10 mg/L and the trend is still respected.  
343 The simulation for the karstic site is particularly interesting as the added years 2011-2015 induce  
344 an inversion of the trend that is well represented by the model. It is also the case for the  
345 limestone site, although the simulation of the last 15 years seems slightly over estimated. In this  
346 case, the decrease of the goodness of fit criterion is related to the extension of a slight bias in  
347 the initial calibration.

348 Overall, the robustness of the model is demonstrated in the three agronomic and geological  
349 contexts. The model was able to simulate in a satisfactory way a 5 years hydrological and nitrate  
350 simulation extension for several systems with different inertia and trends.

351 This point is important to gain the confidence of the decision makers. These simulations validate  
352 the use of the three models for predictive purposes, and by extension, show that BICHE is  
353 suitable for such uses. Decision makers can rely on such predictions, at least on short terms,  
354 without needing to recalibrate the model. However, the model is so easy and fast running (some

355 seconds for 5000 iterations during automatic iteration), that in a normal use, it should be  
356 regularly recalibrated to take the best of the full set of data.

357 Although robust, this type of modelling based on calibration remains dependent on the  
358 characteristics of the input series used during the calibration phase: the input time series must  
359 be sufficiently long and contrasted to obtain a reliable and robust calibration.

### 360 2.5.3 Retrospective analysis on the effect of agronomic measure implementation

361 The last step illustrates a potential operational use of the model to evaluate the impact of the  
362 measures and programs. This evaluation is essential for decision maker who sometimes  
363 question whether the measures taken should be maintained and doubt on their actual  
364 effectiveness. Thus, the model will answer the question “What would have happened if the  
365 environmental measures had not been applied?”

366 The new set of simulations considers continuity of practices as they were before the initiation of  
367 environmental measures (national and local) in those sites. By comparing them to the present  
368 situation, we aim to illustrate and quantify the effectiveness of agronomic measures  
369 implementation on groundwater quality. This scenario has obviously no impact on groundwater  
370 levels and only nitrate comparison will be discussed here (Fig. 3b, 4b, 5b). N balance  
371 comparisons at watershed scale between scenarios have been carried out to help understanding  
372 the different results obtained with the two simulations. The N balance is the comparison between  
373 N input and N output (Oenema, et al., 2003). It was calculated at the catchment scale.

374 For the **basement site**, the new simulation shows a further increase in concentrations. There is  
375 no trend reversal. We can therefore conclude that the observed reversal is due to the change in  
376 practice. The two scenarios are really contrasted. At the end of the simulations, the difference in  
377 nitrate concentration is almost 37 mg/L, the “no measures” simulations reaching 106 mg/L in  
378 December 2015 vs. 62 mg/L.

379 The difference between the 2 scenarios originates from an important land use change from  
380 1989/90, with 40% of the cultivated area converted in meadows before 2007, that yields to a



381 sharp decrease of fertilization (grass is not fertilized) modifying the total N balance. For these  
382 two scenarios, N balances are almost similar from 1985 to 1997 whereas N balances for actual  
383 practices is 45 kg/ha lower in 1997 and around 200 kg/ha lower in 2015 than for “no measures”  
384 scenarios. As the land use transformation was probably progressive, it is difficult to evaluate the  
385 time lag between the action and its effect on groundwater, but the order of magnitude is of 5  
386 years, considering that the first drift between the two curves appears in year 2000.

387 **For the karstic site**, in the “no measures” scenario the increase in concentrations continues and  
388 is confirmed above the threshold of 50 mg/L, whereas the previous simulation showed a  
389 stabilization just below 50 mg/L. Even if the difference between the two scenarios is small in  
390 terms of final concentration (about 10 mg/L), the position of the curve on one side or the other of  
391 the 50 mg/L threshold is of paramount importance, since 50 mg/L corresponds to the drinkability  
392 standard in Europe.

393 The “No measures scenario” N balance and the “Second scenario” N balance are almost similar  
394 from 1985 to 2003 and from 2011 to 2015. But from 2004 to 2010, the “actual practice scenario”  
395 N balance is inferior, with a difference of 64 kg/ha in 2006.

396 The difference between the two scenarios is linked to fertilization efficiency. Between 2003 and  
397 2010, farmers in the catchment were accompanied by the Agricultural Chamber to adjust the  
398 fertilization to each plot (over 80% of the catchment) considering field measurement and  
399 nitrogen modelling use. This use of integrated crop management techniques to optimize the use  
400 of soil and nutrient inputs can be considered the main difference between the two scenarios and  
401 therefore, the major factor affecting the observed nitrate reduction in groundwater (compared to  
402 what it would have been without this effort). The end of the support provided by the Agricultural  
403 Chamber may explain the modification of the N balance and the increase in concentration  
404 observed during the ultimate years. The karstic site, as one could expect, appears as the most  
405 reactive site of the studied sites, due to fast transfer in the vadose zone and extreme  
406 vulnerability of the water table. It may be difficult to exactly define when the measure taken has a

407 significant impact on groundwater, but the order of magnitude, in this karstic example, is after 1  
408 to 2 years.

409 In this karstic site, it is important to notice that the “no measure” scenario does not simulate a  
410 continuous increasing trend as in the other sites, but seems to stabilize on a plateau, except for  
411 seasonal variations. It is therefore conceivable to consider that an equilibrium is reached in the  
412 aquifer system; a permanent mass flow regime which is set up thanks to the short transit times  
413 in the aquifer. Since agronomic input are equal each year, this scenario also evidences the low  
414 influence of the climate on nitrate evolution: despite a succession of contrasted years (640  
415 mm/yr in the hydrologic year 2011-2012, 899 mm/yr in the hydrologic year 2013-2014), the  
416 interannual variation is not visible.

417 **For the limestone site,** the “no measure” simulation drops out the actual simulation as soon as  
418 1995. Unlike in the basement site, the simulation shows an irregular evolution of nitrate  
419 concentration, with a global increasing trend leading to a significant difference at the end of the  
420 simulation of almost 30 mg/L, the “no measures” simulation reaching 121 mg/L in 2015 vs.  
421 93 mg/L.

422 The N balances for “no measure” scenario and the second scenario are almost similar from  
423 1988 to 1992. Since 1992, the “second scenario” N balance is inferior for two reasons. First,  
424 poplars were planted in the vicinity of the well but the area only represents 1% of UAA and  
425 second, the yield increased whereas fertilization was almost stable on the catchment leading to  
426 a more efficient N balance. Therefore, it seems that the improvement of the situation originates  
427 in fertilization efficiency. Over the period 1990-1995, the two scenario nitrate series are almost  
428 identical although voluntary and obligatory environmental and agricultural action plans were  
429 implemented (in 1991 and 1992). A delay of about five years seems necessary before the  
430 impact of actions can be visible. From 1995, the two curves are different although the same  
431 tendencies are preserved.

432 The no measure simulation, repeating the same agronomic input, clearly evidence the climate  
433 impact. In this site, the climatic conditions shape the nitrate evolution in groundwater. The impact  
434 of wet years (as 2000-2001) is probably responsible on the decrease of concentration observed  
435 in 2005-2006. Between 2010 and 2015, the N balance increases because the wheat yield  
436 decreases rapidly but fertilization decreases more slowly (in adaptation of yield decrease)

437 **For the 3 studied sites**, although it may seem theoretical because it probably would have never  
438 happen this way, the retrospective analysis of the “no measure” scenario not only highlights the  
439 impact of the taken measures, but also quantifies the gain in terms of concentration reduction,  
440 estimates delay between measure and impact, and evidence the role of the climate on nitrate  
441 concentration variation in groundwater. In addition, the scenario applied on the three sites  
442 demonstrated that the implementation of programs of measures makes it possible to reduce  
443 nitrate concentrations of groundwater.

444 For 2 of the 3 sites, the measures taken do not yet make it possible to go below the 50 mg/L  
445 threshold, but they have made it possible to reverse the trend of increasing levels with a more or  
446 less significant delay effect depending on the inertia of the system. The key role of  
447 hydrodynamic on groundwater quality trend is also highlighted. These results are critical for  
448 environment managers to decide whether to maintain, strengthen or abandon the measures.

### 449 3 Conclusion

450 This work conclusively shows that the lumped model BICHE was able to correctly simulate the  
451 long term trends of both water and nitrate evolutions in three different hydrogeological and  
452 agricultural contexts. By contrast, due to the monthly time step of input data (adapted to input  
453 data uncertainty - e.g. real fertilization) and simplifications inherent to lumped models, short-term  
454 variations were less correctly reproduced. The lack of detailed agronomic data often leads to  
455 the use of rough approximations or input of data from communal or departmental statistics,  
456 which can span over larger areas than the catchment. However, in a perspective of environment

457 management, the need is to get simple tools to simulate and extrapolate trends and trend  
458 reversal, under agronomic and climatic scenarios. The BICHE lumped model is therefore well  
459 suited for such a purpose.

460 For the three sites, a validation exercise conducted using an extension of 5 years of the dataset  
461 proved successful. The hydrological simulation was improved and the nitrate concentration  
462 simulation was barely altered proving the robustness of the calibration process. Besides, thanks  
463 to the relatively limited number of parameters and the automatic calibration, the use of the  
464 BICHE model is very fast (it runs within seconds on standard computers). Lastly, the  
465 retrospective analysis of effects of implementation of agricultural practices highlighted the ability  
466 of this tool to support the evaluation of programs of environmental measures. The “what if”  
467 scenarios have an educational power useful to make stakeholders (particularly farmers)  
468 understand that their efforts to reduce agricultural inputs are not in vain and politician that  
469 environmental measures are worth trying.

470 The results of the “what if” scenario undertaken in this work show that the agricultural policies  
471 enforced in France had an impact in three contrasted climate and agricultural sites, that can be  
472 more or less delayed in time.

473 Unquestionably, BICHE can be used operationally for decision maker purposes, outside a  
474 research framework. Beyond retrospective analysis, this tool could be used in a prospective  
475 purpose to support discussion between farmers and stakeholders in order to implement new  
476 programs of measures. The model will be useful to determine the extent of efforts to be made  
477 and to estimate the time lag between the implementation and the effect on groundwater quality.

478

## 479 [Acknowledgments](#)

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553

## Figure Caption

Figure 1: Diagram of the BICHE model

Figure 2: Location of the three studied sites on the hydrogeological map

Figure 3: Time-series of piezometry (A) and nitrate concentration (B) for the basement site: observation (real data), calibration (dataset until 2010), validation (extended set of five years (2011-2015) without any new calibration process compared to “calibration”), no measure (continuity of practices as they were before the initiation of environmental program of measures)

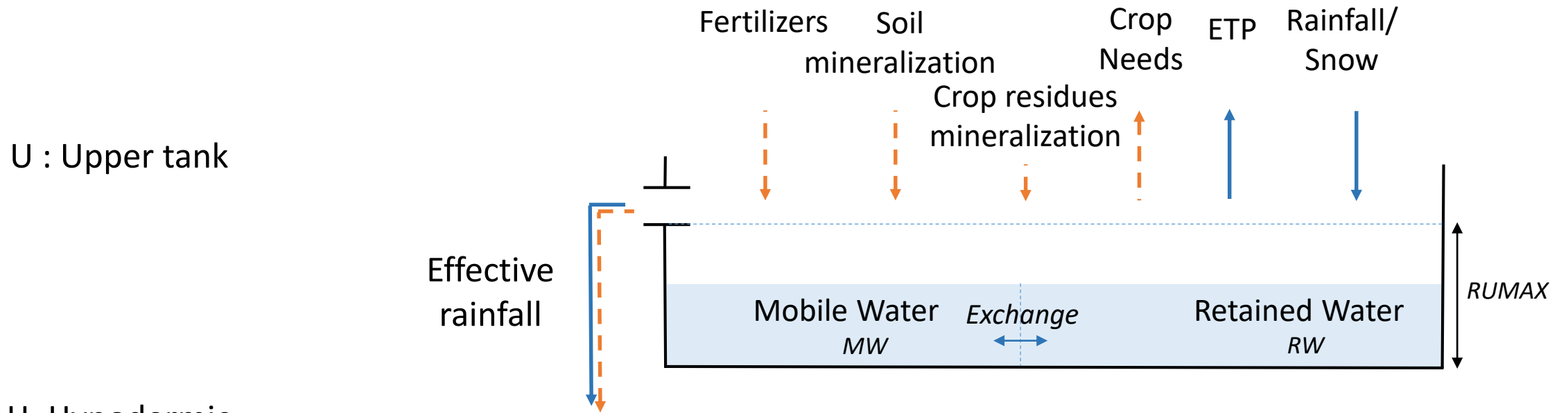
Figure 4: Time-series of piezometry (A) and nitrate concentration (B) for the limestone site: observation (real data), calibration (dataset until 2010), validation (extended set of five years (2011-2015) without any new calibration process compared to “calibration”), no measure (continuity of practices as they were before the initiation of environmental program of measures)

Figure 5: Time-series of piezometry (A) and nitrate concentration (B) for the karstic site: observation (real data), calibration (dataset until 2010), validation (extended set of five years (2011-2015) without any new calibration process compared to “calibration”), no measure (continuity of practices as they were before the initiation of environmental program of measures)

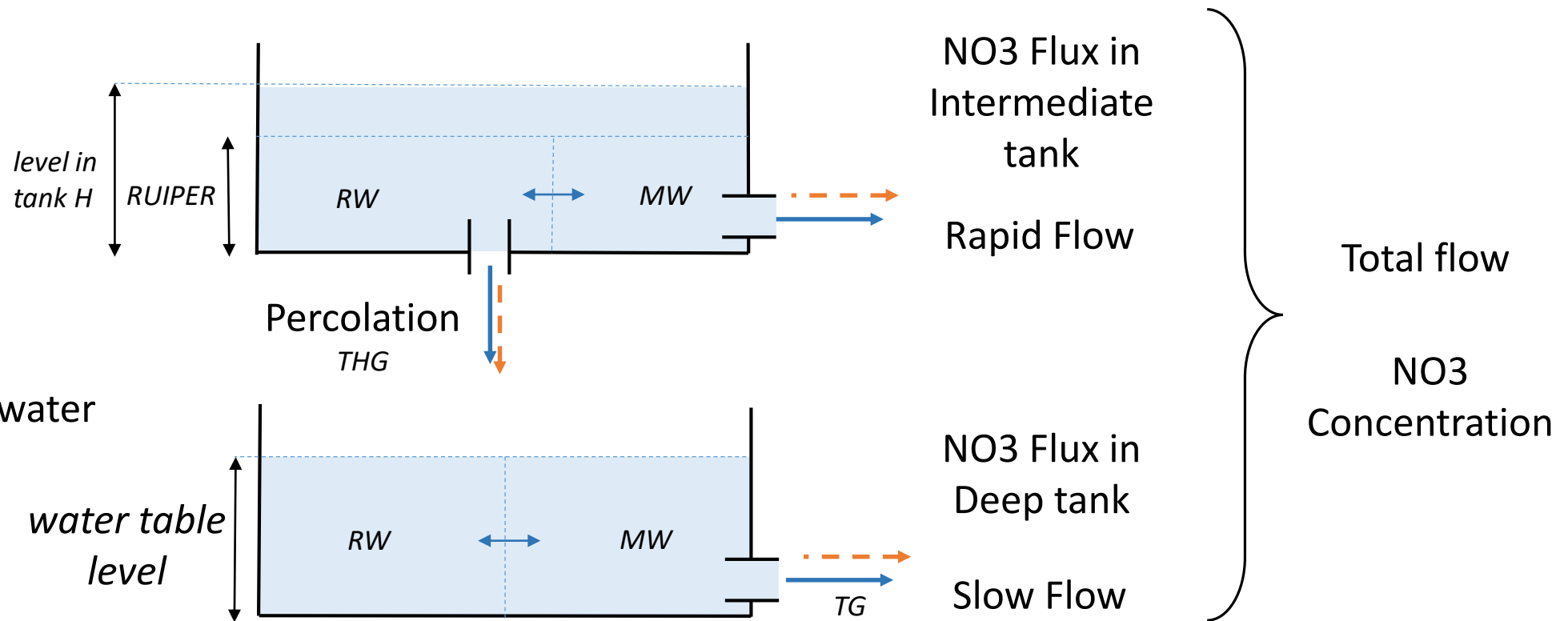
## Table caption

Table 1 : Studied catchments presentation





H: Hypodermic tank



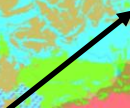
***Basement site***



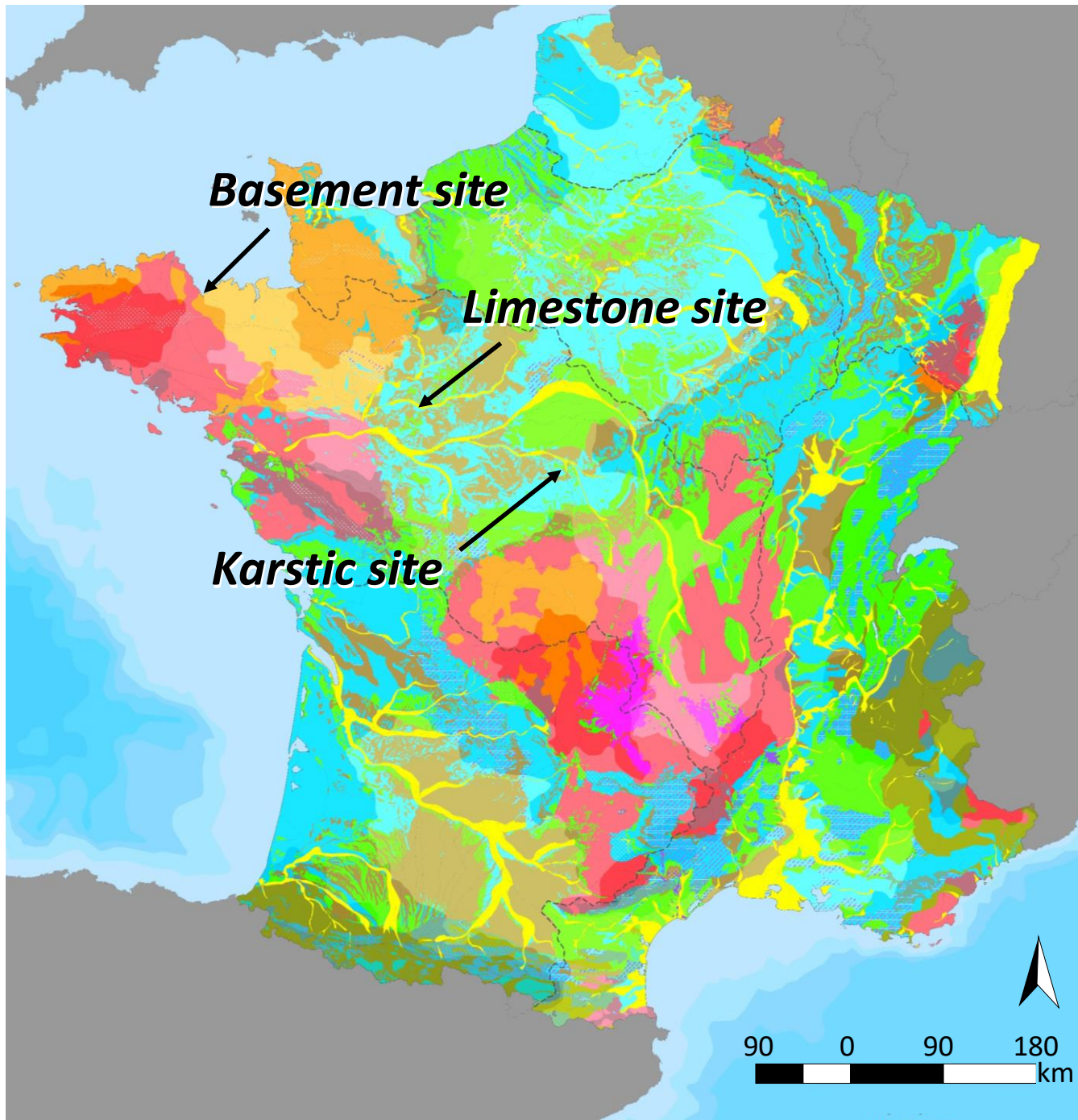
***Limestone site***

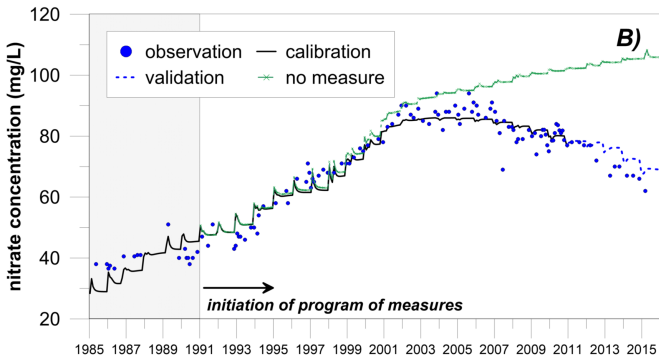
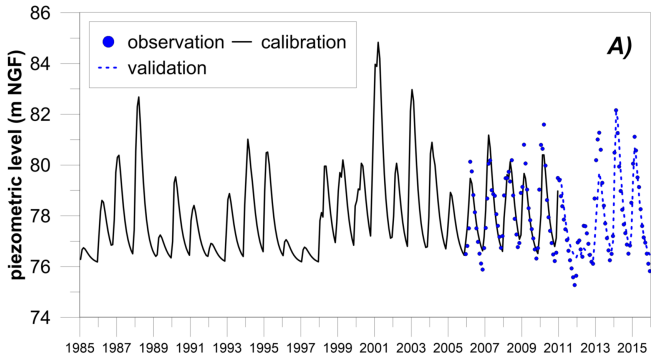


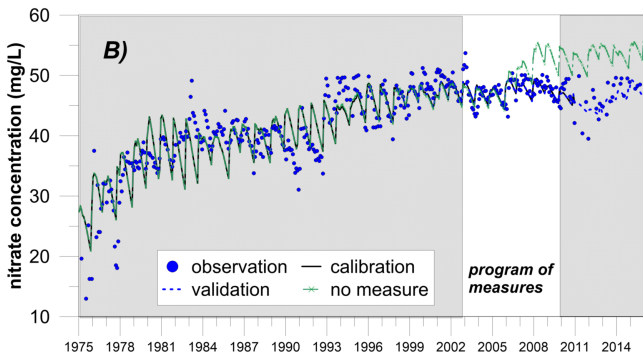
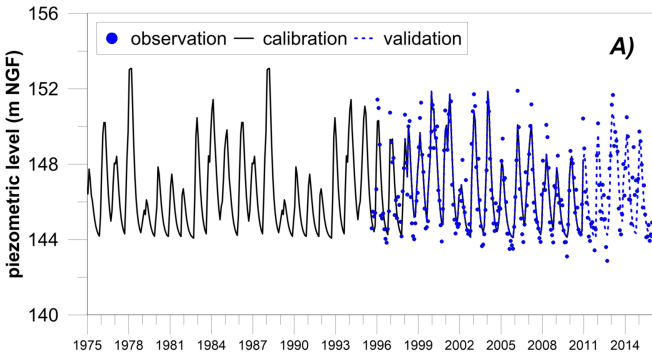
***Karstic site***

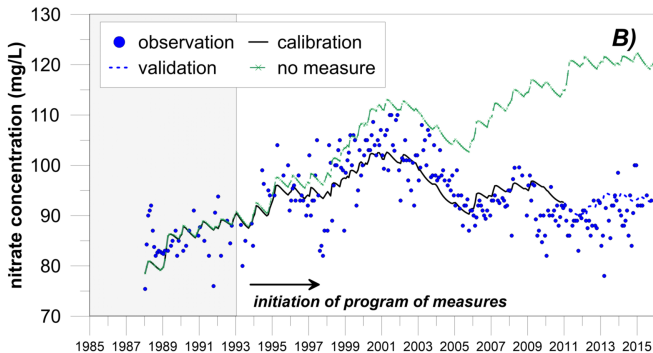
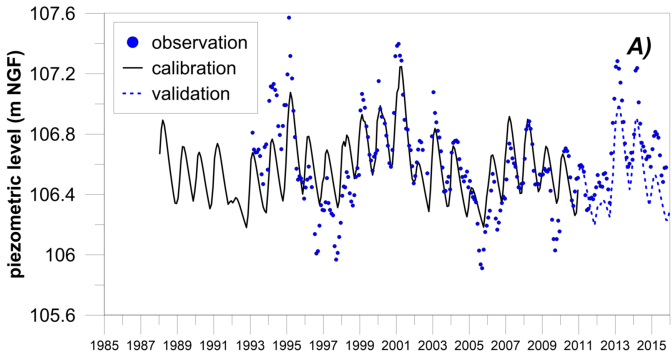


90 0 90 180  
km









1 Table 1 : Studied catchment presentation

	BASEMENT SITE	KARSTIC SITE	LIMESTONE SITE
Catchment municipality (NUTS3)	Plourhan	Déols	Pentvert
Region (NUTS1)	Brittany	Centre-Val de Loire	Pays de la Loire
Station coordinates (WGS84)	48.6400 ; -2.8970	46.8287 ; 1.7235	48.3279; 0.2660
Closest major town	Saint-Brieuc	Chateauroux	Le-Mans/Alençon
Catchment area surface	0.6 km <sup>2</sup>	50 km <sup>2</sup>	9 km <sup>2</sup>
Altitude mean	100 m	150 m	125 m
average slope	1%	0.25%	0.25%
Geologic formation	Basement formation	karstified limestone	fissured limestone
Soil average thickness	40-80 cm	20-80 cm	45 cm
Water Holding Capacity (mm)	100	100	50
Average yearly rainfall (mm/yr)	767	729	699
Particularly wet years	1998 to 2003	1987; 1993; 1999-2000	1992-93, 1998-2000, 2006
Particularly dry years	1988, 1990, 1995-96, 2004	1988-1990, 2004	2004
Average yearly PET (mm/yr)	688	846	739
Major Nitrates concentration increase in groundwater	In the 1990s and before 1985	In the 1970's	Before 1985
Major Land use change between 1985 and 2010	Growth and decrease of vegetables surfaces, maximum in 1995 then main fallow	Mainly wheat in rotation with rapeseed. Rather constant land use over 1985-2010	Corn surface decrease in favour of rapeseed between 91 and 2007. Decrease in meadow surface between 93 and 2003
Inertia of hydrologic system	Not very-reactive	Very reactive	mixed

2

3