Comparison of 1D and 2D modelling of pesticide transfer in a tile-drained context. Application to la Jaillière site.

Romain Dairon, Nadia Carluer, A. Dutertre, B. Real, Françoise Leprince

To better reflect its missions, Cemagref becomes Irstea.

Comparison of 1D and 2D modelling of pesticide transfer in a tile-drained context.

Romain Dairon[a*] Nadia Carluer[a], Alain Dutertre[b], Benoit Real[b], Florence Leprince[b].

a. Irstea, UR HHLY, 5 rue de la Doua, 69100 Villeurbanne, France (*corresponding author: romain.dairon@irstea.fr),

b. Arvalis-Institut du végétal, 3 rue Joseph et Marie Hackin 75016 PARIS.

Introduction & Objectives

▪ **General guideline** : European Water Framework Directive (2000) ➔ Reduce pollutant in water. In France : ECOPHYTO (2008-2018) ➔ reduce amount of pesticide used by 50 %.

▪ **One dimensional models** : widely use in regulation procedure for pesticides leaching in U.E : MACRO, PEARL, PRZM *(FOCUS 2001)*.

▪ **Context** : in tile drained soils, the drained water dynamic affects transport of water and solute in soils. Preferential flow is also recognized as a key process for pesticide exportations in structured soils (e.g, Jarvis, 2007).

▪ **Our objectives** :

- Estimate the role of the drained water table and preferential flow in pesticide fate.
- Evaluate advantages, disadvantages and efficiency of MACRO and HYDRUS-2D using a long term validation period.

1-Field description

▪ The site of la Jaillière is an European reference for drained soils (Fig.1), and used for homologation.

▪ Located in North West of France. The climate is temperate oceanic with 705 and 724 mm of precipitation and potential evapotranspiration, respectively.

▪ Long term monitoring for water (1987-2013), Nitrate (1988-2013) and pesticides (1994-2013).

▪ Short step data for bromide and two pesticides :
-Diflufenican (DT50 = > 140 d, Koc = 2000 L.Kg^{-1})
-Isoproturon (DT50 = 15 d, Koc = 124 L.Kg^{-1})

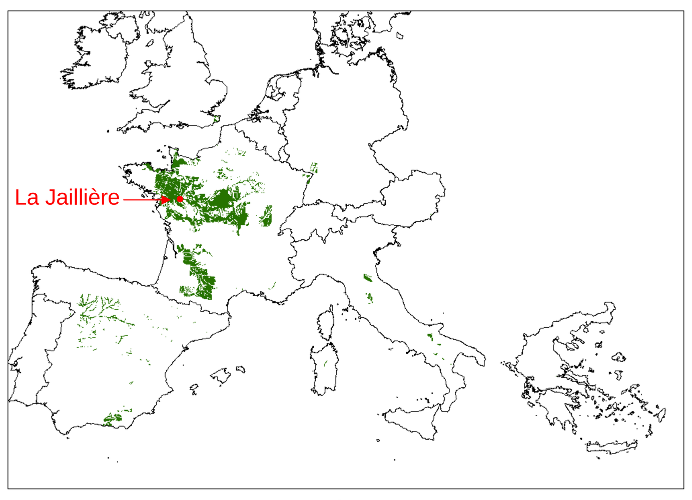


Fig. 1 : Location of the site of la Jaillière and distribution of this drainage scenario (D5) in Europe (FOCUS, 2001).

Tab. 1 : Main soil characteristics of the plot T4.

Horizon	Thickness	Clay (%)	Silt (%)	Sand (%)	O.M (%)^{a}	Bulk density (g.cm3)	pH (water)	Structure
Ap	30	20.8	44.6	34.6	2.17	1.55	6.3	Blocky
E	18	25.9	41.3	32.8	0.77	1.63	7	Blocky
Bt	17	49.2	35.3	15.5	0.46	1.7	5.6	Prismatic
Bt/C	45	42.7	35.8	21.5	0.36	1.7	4.9	Blocky

▪ Corn-winter wheat rotation with conventional tillage.

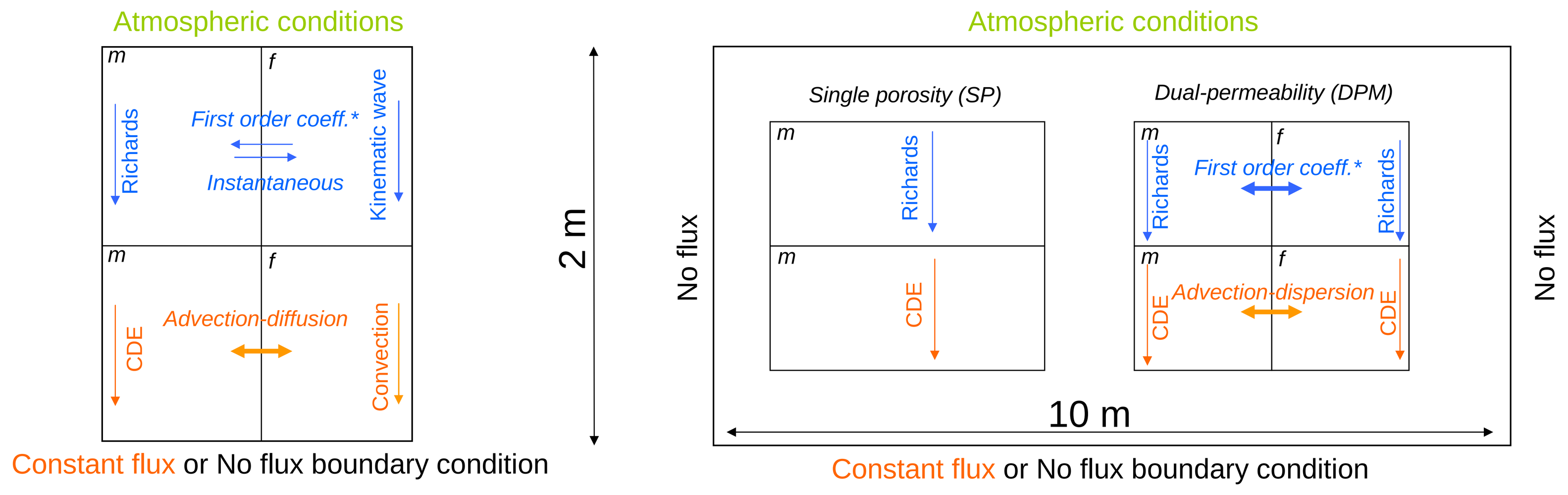
▪ Drained (0.9 m deep and 10 m spacing) Stagnic luvisol located on a flat plateau.

▪ Visible fractures, earthworms burrows and roots channels on the field (photo 1).

Photo 1 : Fractures at the soil surface, April 2013.

2- Models descritpion & Methodology

MACRO 5.2 (Larsbo & Jarvis, 2003) — **HYDRUS-2D (Simunek & al, 2012)**



Initial condition : 6 months « blanks » simulation for 2005-2006. For the validation step, continuity was assumed between years (water and solutes).

Upper boundary : Hourly rainfall. Evaporation and transipiration rate calculated by MACRO and also used by HYDRUS. Water and solute enter into matrix domains.

Parametrization

Hydrodynamics parameters estimate by pedotransfer function. We used FOOTPRINT pedotransfer function for both dual permeability models as HYDRUS-2D do not provide such data.

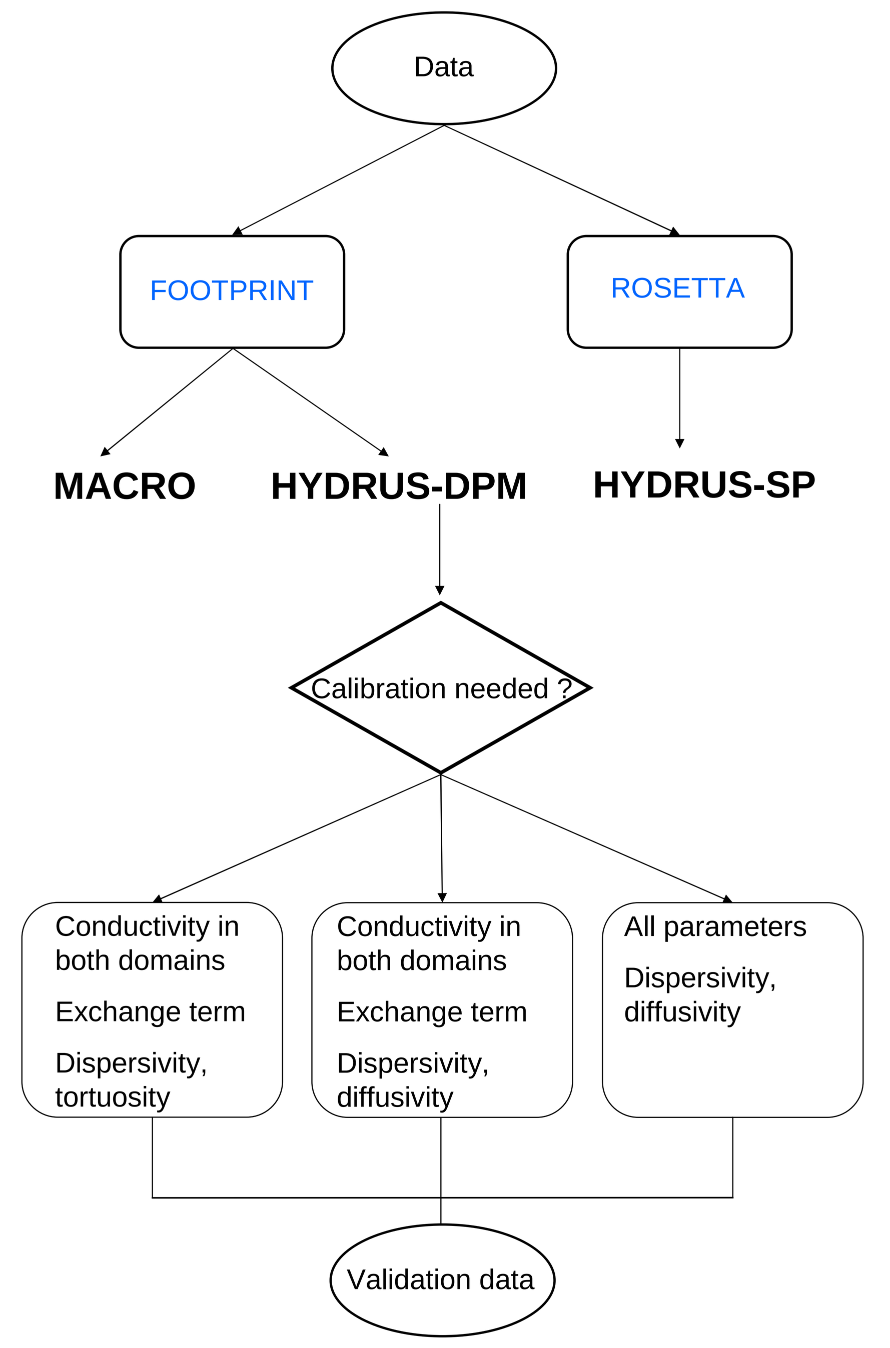
Initial simulations are compared with data. If needed, sensibilty analysis was performed to determine key parameters to fit.

Calibration

Inverse solution was used for the simple porosity model. For dual permeability models, we decided to calibrate only few parameters based on sensibility analysis.

Validation

Validation was perfomed on a 10 years period for water, isoproturon (IPU) and diflufenican (DFF).



3- Results & discussion

DATA

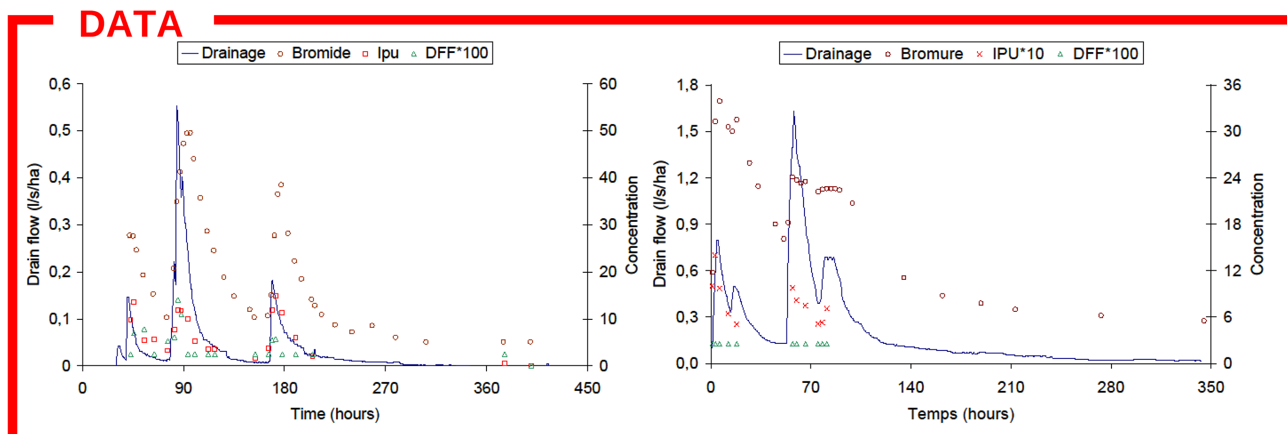


Fig. 2 : Measured drained flow and bromide, isoproturon, diflufenicanil concentrations during two periods : (left) Following application (december) and (right) During the intensive drainage season (february). Concentrations are expressed in mg.L^{-1} for bromide and µg.L^{-1} for pesticides.

Bromide lag behind peak of drainage following application and is simultaneous with drainage during the itensive drainage season (IDS).

Pesticides peaks are ahead drainage and bromide peaks in both season.

➔ Does the drain water table dynamic influence pesticides exportations ?

Simulation

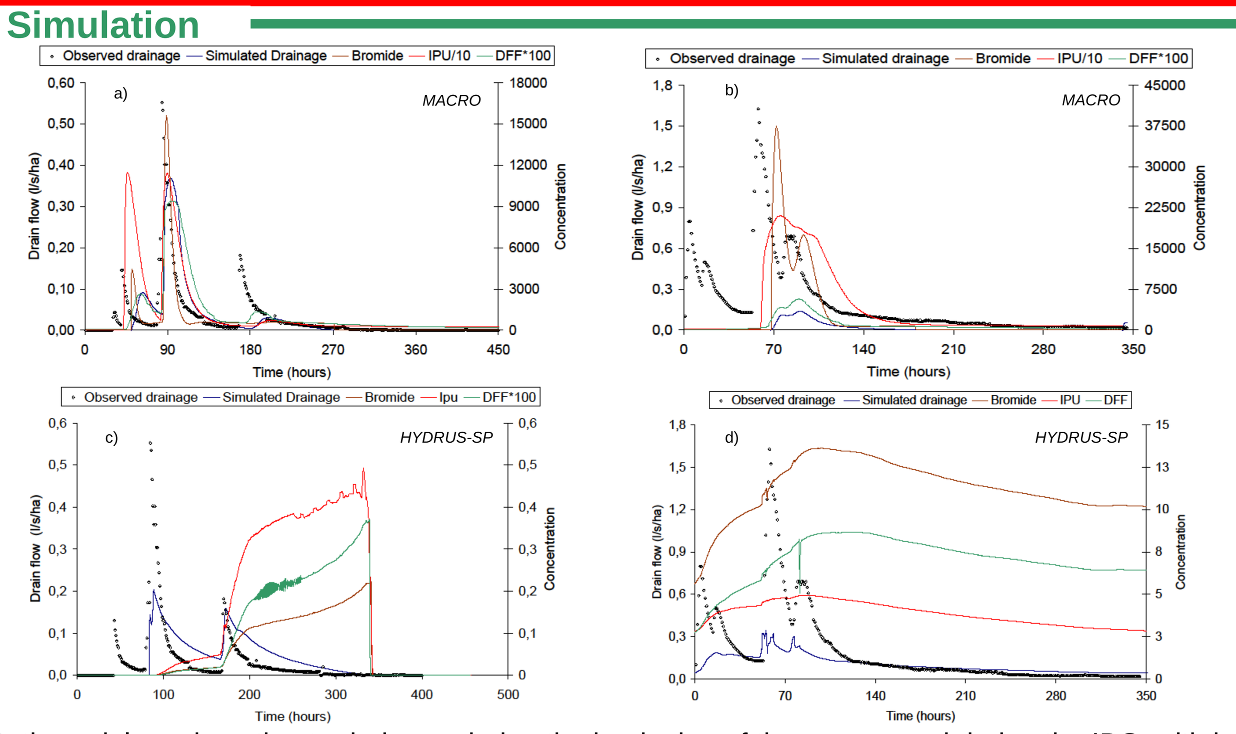


Fig. 3 : Simulated drainage and bromide, IPU, DFF concentrations following application (a) and during the IDS (b) for ***MACRO*** *(c) and* ***HYDRUS-SP*** *(d). Concentration are expressed in mg.L^{-1} for bromide and µg.L^{-1} for pesticides.*

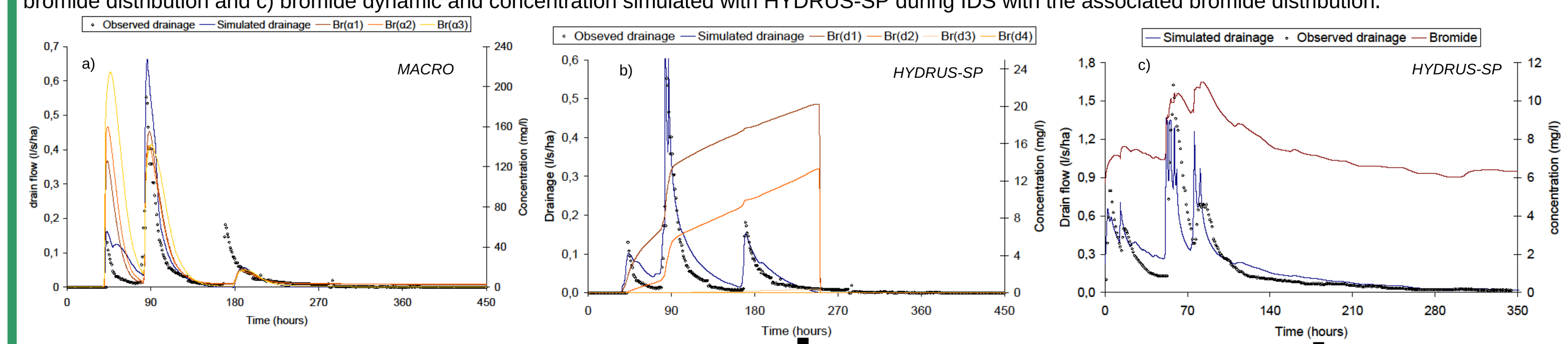
▪ Both models underestimate drainage during the beginning of the season and during the IDS, with initial parameters.

▪ **MACRO** overestimates concentration of all solutes following application and during IDS.

▪ Inverse problem is observed for **HYDRUS-SP**. Concentrations increase with time until the beggining of the IDS (fig. 3d).

CALIBRATION

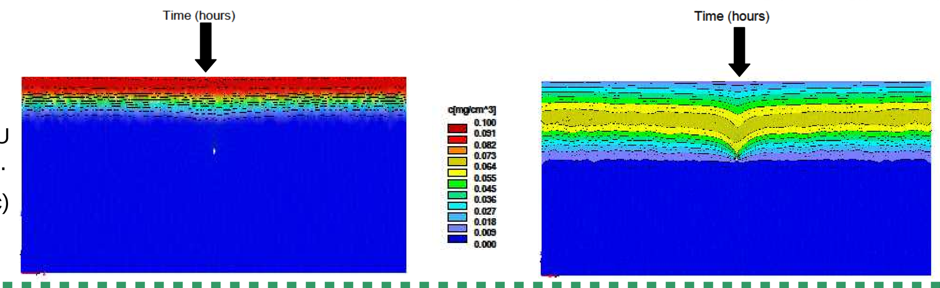
Fig. 4 : Bromide dynamics and concentrations for different values of the a) mass transfer coefficient in MACRO, b) dispersivity in HYDRUS-SP with the associated bromide distribution and c) bromide dynamic and concentration simulated with HYDRUS-SP during IDS with the associated bromide distribution.



Both models correctly simulate drain flow (Fig. 4a,b,c).

MACRO can't describe bromide dynamic following application (Fig. 4a). However, once calibrated, concentrations are in the ranged of data for bromide and IPU for the two periods of monitoring, yet underestimate for DFF.

HYDRUS-SP partly represents bromide dynamic(Fig. 4b, 4c) but concentrations are still increasing following application. Predicted pesticide concentrations are low



VALIDATON

Tab. 2 Drainage (Dc),isoproturon and diflufenican cumulated flux simulate by MACRO and HYDRUS-SP compared to the 10 years data. Data in ***bold*** *represent acceptable results. Simulated data in blue and orange fail to predict water and solute, respectively.*

Year	Data			MACRO						HYDRUS-SP					
				Initial parametrization			Calibrated			Initial parametrization			Calibrated		
	D_c (mm)	IPU_c (mg/ha)	DFF_c (mg/ha)	D_c (mm)	IPU_c (mg/ha)	DFF_c (mg/ha)	D_c (mm)	IPU_c (mg/ha)	DFF_c (mg/ha)	D_c (mm)	IPU_c (mg/ha)	DFF_c (mg/ha)	D_c (mm)	IPU_c (mg/ha)	DFF_c (mg/ha)
1995	500	-	-	**403**	0	0	**434**	-	0	156			Does not converge		
1996	109	1449[a]	95[a]	**128**	11790	0	**141**	**1436**	2	85	3	0	**71**	6	2
1997	165	-	4	**171**	3	0	**189**	0	18	93	0	**9**	27	0	**3**
1998	193	No data[a]	4	**233**	560	34	**252**	**68**	270	104	1	**3**	121	2	**2**
1999	290	-	-	**327**	5	124	**354**	0	307	202	0	1	149	0	0
2000	382	5364[a]	0	**311**	20000	74	**336**	**2059**	198	156	0	1	181	15	0
2001	512	-	-	**509**	85	83	**546**	16	196	246	0	0	255	0	0
2002	144	632[a]	0[a]	**208**	5184	32	228	**791**	46	84	1	0	68	1	12
2003	329	-	0	185	1	11	205	0	15	90	0	0	55	0	2
2004	236	2131[a]	228[a]	**231**	23510	5	**248**	**2247**	25	95	10	1	Does not converge		
2005	10	-	0	75	0	12	92	0	3	29	0	0	**0**	0	0
2006	121	1016[a]	8.5[a]	**122**	127500	**28**	**125**	**210**	20	78	2	1	**103**	0	**27**

Drain flow : Cumulated drainage is reasonnably well predicted by **MACRO** with or without calibration. However, Nash-Sutcliffe coeffecient (between 0.2 and 0.7) and analysis of hourly data (not shown here) shows understimation of simulated drain flow during IDS for all campaigns. **HYDRUS-SP** underestimate cumulated drainage due to overestimation of transpiration and runoff.

Solute : **MACRO** and **HYDRUS-SP** do not match Isoproturon exportations and fail to predict DFF exporations during the campaign following application without calibration. Once calibrated **MACRO** matchs well IPU losses and overestimates long term exporation of DFF; **HYDRUS** does but this is due to a really slow migration. For the same reason HYDRUS simulate low IPU exportation due to higher degradation rate.

HYDRUS-DPM

Some problems occurred in the last week concerning upper boundary conditions. We realized that the parameter governing repartition of water and solute between matrix and fractures was stuck. Thus, all solute and water got in macroporosity and change flow and flux dynamics. We solve the problem (thanks to J.Simunek) but others problems have happened since.

Conclusion & perspectives

Solute transport : it's seems that pesticides are mainly transport by macroporosity in our soils. HYDRUS-DPM results will certainly give some additional proofs.

▪ **MACRO** : give acceptable results for water, and once calibrated for Isoproturon. Problem to correctly simulate pestistant and strongly sorbed component ➔ A need for some chemical processes representation.
Some code problems in this version (tillage, kinetic sorption).

▪ **HYDRUS-2D** : can be used to represent complex problems ➔ Yet convergence problems is time consuming (no bug report). Dual-permeability need 17 parameters (for water) which can lead to some convergence and equifinality problems. No roots and crop evolution in some layers. ➔ problematic for validation procedure. However HYDRUS can certainly provide significant informations on water and solutes processes.

▪ **Next steps** :
1- Compare initial and calibrated results with simulations using field and laboratory data : Conductivity and retention curves, phyisico-chemicals key parameters in each layer.
2- Use both physical and chemical non-equilibrium to account for formation of bound residues in soils and sorption kinectics.

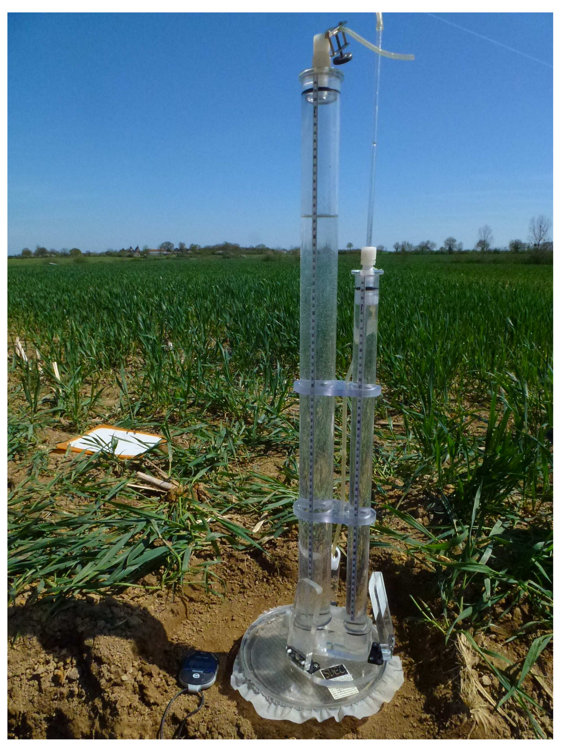


Photo 2 : Tension Disc infiltrometry on the surface plough layer. April 2013.

Acknowledgements : The authors thank *Bruno Cheviron* for his help in coupling PEST with MACRO.

Reference :
Focus (2001). FOCUS surface water scenario in the EU evaluation process under 91/414/EC.
Jarvis, N. J. (2007). "A review of non-equilibrium water flow and solute transport in soil macropores: principles, controlling factors and consequences for water quality." European Journal of Soil Science 58(3): 523-546.
Larsbo, M. and N. Jarvis (2003). MACRO 5.0. A model of water flow and solute transport in macroporous soil, Swedish University of Agricultural Sciences.
Simunek, J. and M. Sejna (2011). HYDRUS Technical Manuel Version2. Software Package for Simulating the Two- and Three-Dimensional Movement of Water, Heat and multiple Solutes in Variably-Saturated Media. Prague, Cz Republic, Pc Progress: 230.

Pesticide Behavior in Soils, Water and air. 2-4 september 2013, York Univsersity (UK)