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Towards operational models for water and pesticide fluxes at the catchment scale: model performance vs. data quality

Bouvet L., Louchart X. , Voltz M.

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Project context



Pesticide pressure on surface waters

Optimal reduction needs decision support tools



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Developping tools to
**STUDY, DIAGNOSE &
ADVISE**

Modelling objectives

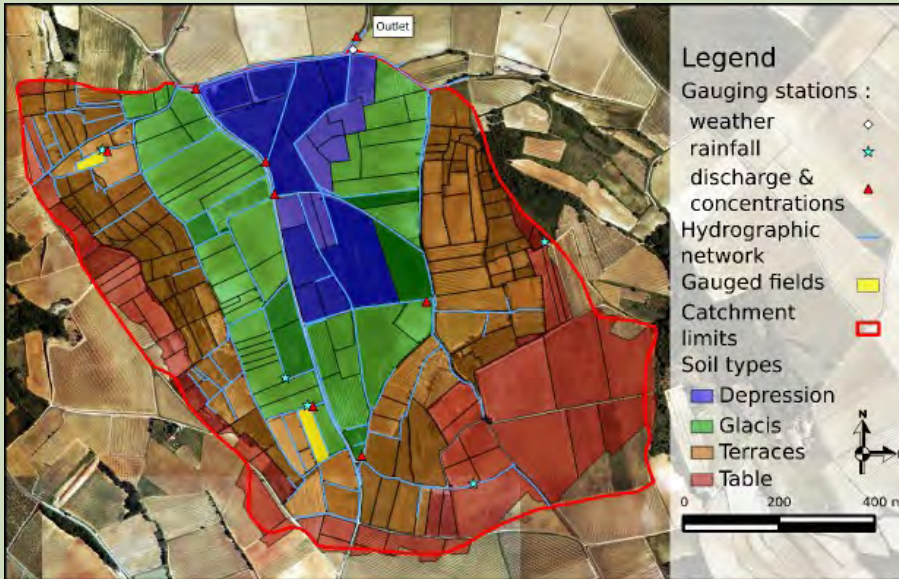
Develop a distributed hydro-chemical modelling for agro-hydrosystems

Evaluate the influence of human practices (spatio-temporal distribution of applications, soil management, anthropogenic features)

Evaluate the model performance vs. input data quality

Material & methods

The Roujan catchment



91 ha

Sub-humid mediter-ranean climat

Hortonian overland flow

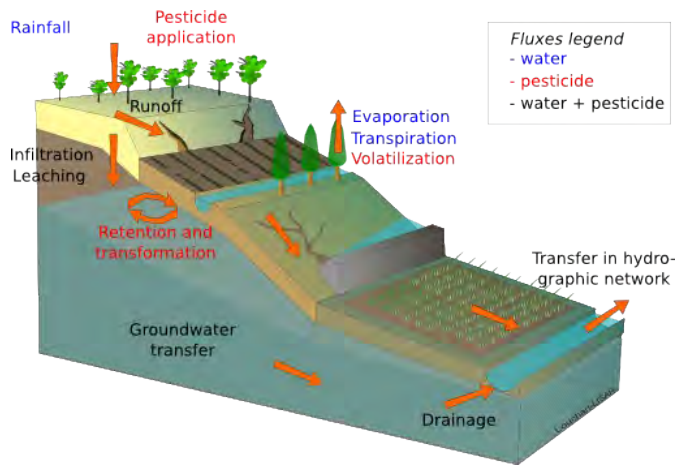
13 km ditch / km²

⇒ highly reactive

Land use : 50 - 80% vineyards

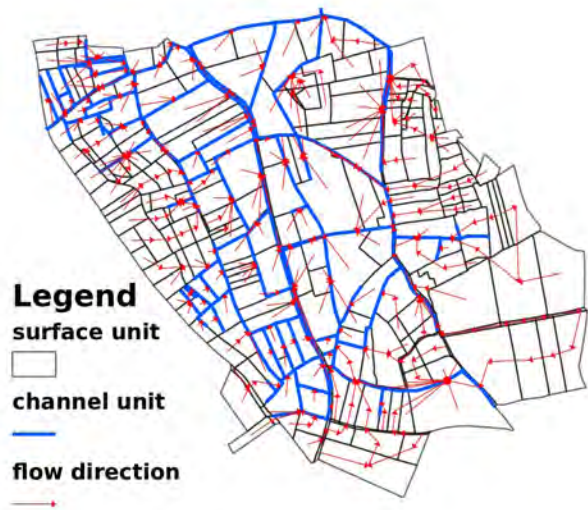
⇒ herbicides & fongicides on bare soils

The MHYDAS model



Pesticide processes:

- applications: soil/foliage partition according to pesticide, ground cover, material & setting
- Pesticide dissipation: 1st order kinetic
- foliar washoff (rainfall threshold)
- mobilisation:
 - instantaneous & uniform mixing in the mixing layer
 - K_d increases with time (cf. aging)
- advective transfer through overland and channel water flow



Model parameterisation

Input data common to all scenarios

Parameter	Data source	Estimation method
<i>land use</i>	<i>field data</i>	<i>typology</i>
geometry & topology (surface & channel units)	DEM + cadastres + aerial images + land use	GIS (GeoMHYDAS)
soil infiltrabilities: f_c , f_o	simulated rainfall + land use	typology of f_c / land use $f_o = x \cdot f_c$
Pesticide properties (DT50, Koc, Kd aging, solubility)	Louchart & Voltz (2007)	--
mixing layer thickness	Leonard <i>et al.</i> (1987)	--
Pesticide application info (molecule, date, dose, field, material)	interviews with farmers	--

Model parameterisation

Input data specific to each scenario

scenario n°	Pilot site	Non-pilot site	
	1	2	3
rainfall	3 tipping buckets	cumulative rainfalls for 6 minute time step (Météo-France© data type)	
soil textures	soil map (1:5,000)	soil map (1:,25,000)	soil map (1:100,000)
characteristic soil moistures	soil texture + PTF	soil texture + PTF	
soil BD & OC	soil map + land use + soil texture	typology of BD & OC based on land use + soil texture	

⇒ influence of rainfalls and soil characteristics accuracies on model performances

Hydrologic calibration

Automated individual rainfall-event calibration:

- PEST program (Doherty, 2005)
- Gauss–Marquardt–Levenberg algorithm

Calibrated parameters:

- mean overland & channel flow celerities
- initial soil water content
- channel infiltration coef.
- f_0/f_c ratio

Observed data:

- water discharge at the catchment outlet

Calibration criteria:

- NS efficiency index
- RE on V_{tot} & Q_{max}

Pesticide calibration

Individual rainfall-event calibrated parameters:
values and ranges

Parameter	Diuron	Oryzalin	Simazine
DT ₅₀	90 [20 - 180]	20 [15 - 50]	60 [20 - 150]
Koc	480 [400 - 500]	600 [500 - 1200]	130 [10 - 300]
Kd aging	0.21 [0.05 - 5]	0.30 [0.05 - 5]	0.29 [0.05 - 5]

Observed data:

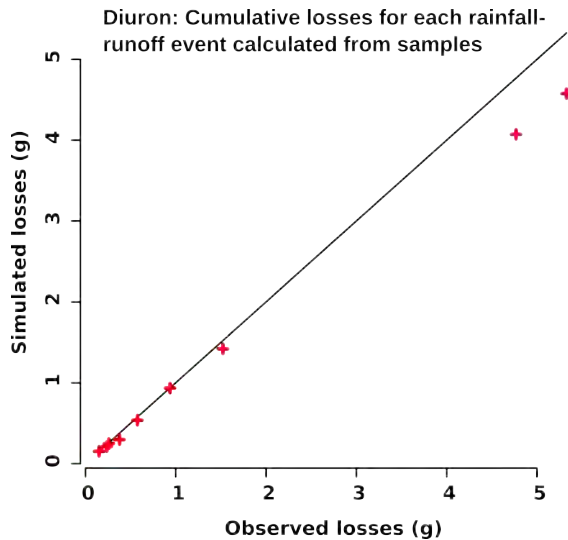
- pesticide concentrations from simple & grab samples (water flow variations dependent)

Calibration criteria:

- MSE for pesticide fluxes at sampling date
- SE for the sum of pesticide fluxes at sampling date

Results & discussions

Pilot site scenario



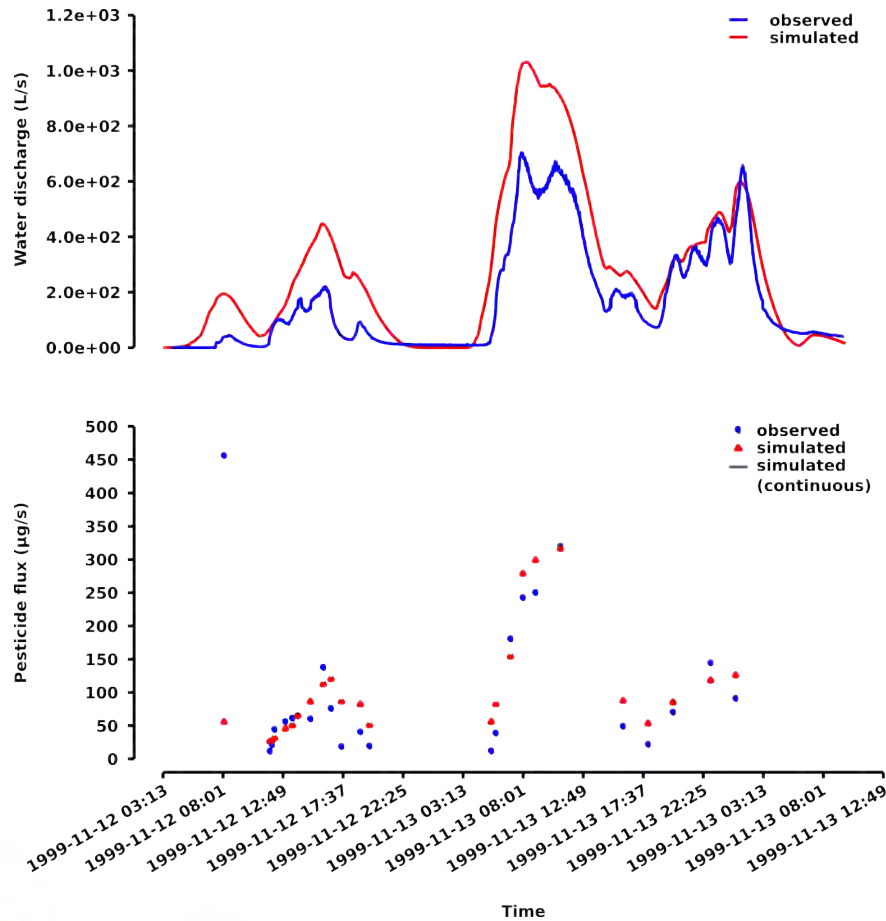
Diuron Sim/Obs cumulative losses ratio

	min	max	mean	std
samples	0.79	1.00	0.91	0.07
event	0.53	17.30	5.00	5.24

Calibration performances:

- nice fit between simulated & observed cumulative losses at sampling dates
- 2 poor performances:
 - event 2 days after diuron application
 - bad hydrologic simulation
- when comparing simulated and estimated mean losses per event : bad results
 - ↳ influence of sampling representativity

Pilot site scenario



Calibration performances:

- nice fit between simulated & observed fluxes dynamics

⇒ good representation of main processes

Pilot site scenario

Diuron parameters' values without outliers

Parameter	min	max	mean	std
DT_{50}	62	88	75	8
K_{oc}	427	500	487	27
K_d aging	0.24	0.74	0.41	0.16

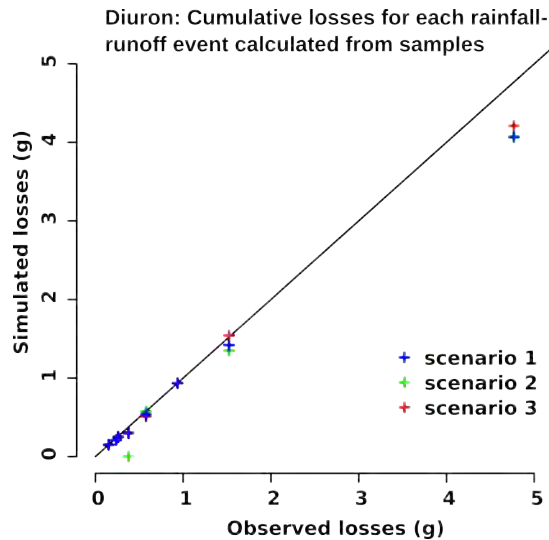
Diuron parameters' values for outliers

Parameter	1999-05-17	1999-08-02
DT_{50}	180	180
K_{oc}	500	500
K_d aging	1.06	0.33

Parameters' values

- rather homogeneous parameter values
- K_{oc} upper bound / soil OC fraction under-estimated ?
- 2 outliers:
 - 1999-05-17:
 - 2 days after diuron application
 - 1999-08-02:
 - undeclared application ?
 - local minimum ?

Non pilot site scenarios



Diuron Sim/Obs cumulative losses ratio

scenario	min	max	mean	std
1	0.79	1.00	0.91	0.07
2	0.00	1.00	0.83	0.32
3	0.81	1.01	0.92	0.08

Calibration performances:

- results equivalent to pilot site
- worst performances: same reasons
- same sensitivity to sampling representativity

Non pilot site scenarios

Diuron parameters values

scenario	Parameter	min	max	mean	std
1	DT_{50}	62	180	98	47
1	K_{oc}	427	500	490	24
1	K_d aging	0.24	1.06	0.47	0.26
2	DT_{50}	20	180	103	61
2	K_{oc}	400	500	475	43
2	K_d aging	0.21	2.65	0.83	0.72
3	DT_{50}	20	180	95	66
3	K_{oc}	400	500	478	44
3	K_d aging	0.48	2.65	0.89	0.89

Parameters values

- DT_{50} similar mean values
- K_d aging much higher
- more outliers & variability
- ⇒ OC parameterisation ?
- ⇒ local minima ?

Conclusions & perspectives

Conclusions

- good simulation performances in comparison to previously published model evaluations
- importance of choosing the calibration & performance evaluation criteria according to sampling strategy
- reasonable soil & rainfall data scarcity
 - does not seem to affect too much pesticide simulation performances
 - parameter values variability is increased probably due to OC parameterisation & calibration strategy

Perspectives

- multi-events calibration & validation of the pesticide module
- evaluate the pesticide module on a larger rainfall-runoff event data-base
- input data-scarcity scenarios for pesticide application related data (date, dose, area)
- multi-scales model evaluation

References

Doherty, J. 2005. PEST, Model-Independent Parameter Estimation, User Manual: 5th Edition. Watermark Numerical Computing

Leonard, R., Knisel, W., Still, D. 1987. Gleams: Groundwater loading effects of agricultural management systems. Transactions of the ASAE, 30, 1403-1418

Louchart, X. & Voltz, M. 2007. Aging effects on the availability of herbicides to runoff transfer. Environmental Science & Technology, 41, 1137-1144

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INRA

Thank you for your attention

Contact:

lionel.bouvet@envilyls.com

lionel.bouvet@supagro.inra.fr

web:

<http://www.envilyls.com>

<http://www.umr-lisah.fr>

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