New insight into pesticide partition coefficient K_d for modelling pesticide fluvial transport with the SWAT model

Laurie BOITHIAS, Sabine SAUVAGE, Raghavan SRINIVASAN, Jeff ARNOLD, José-Miguel SANCHEZ-PEREZ

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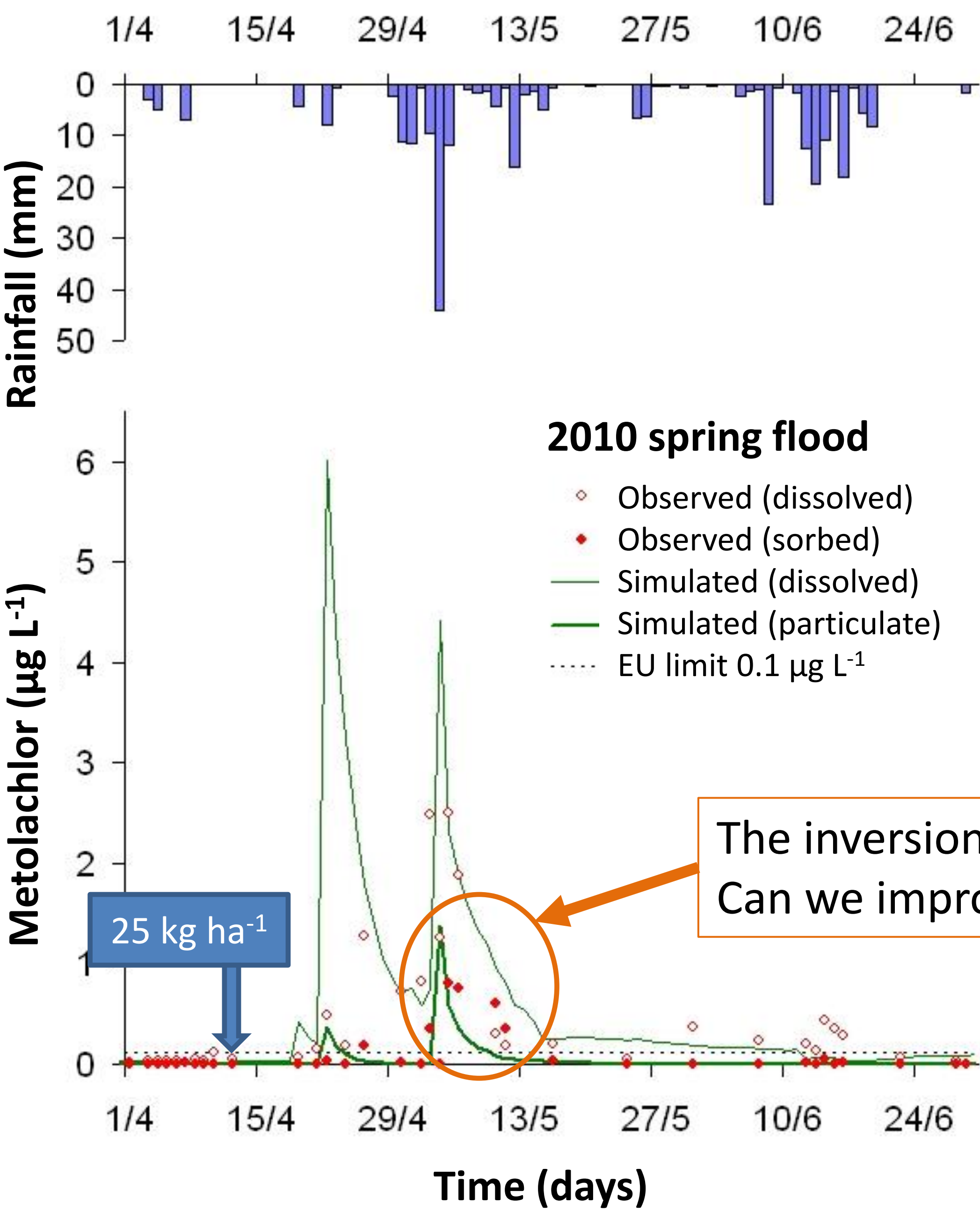
Pesticides and floods

-Surface water pesticide contamination is an issue for ecosystems and human consumption (0.1 – 0.5 µg L^{-1} for drinking water)

-Floods play a major role in pesticides transfers : e.g. 61% metolachlor / 17% time (Boithias et al., 2011)

-Managers need reliable predictive tool

Pesticide partition modelling in SWAT



Case of **metolachlor**:
pre-emergence herbicides
S_w = 480 mg L^{-1}; log K_{ow} = 2.9

The inversion of the partition is not simulated.
Can we improve it ?

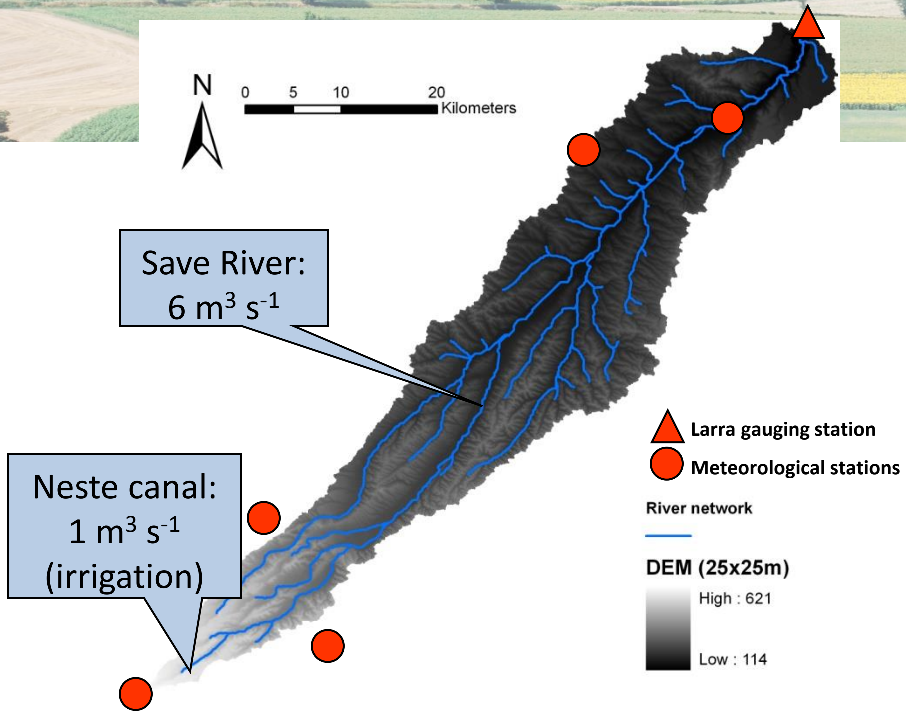
Boithias et al., J. Hazard. Mater., 2011,
Boithias et al., Region. Environ. Change, In revision

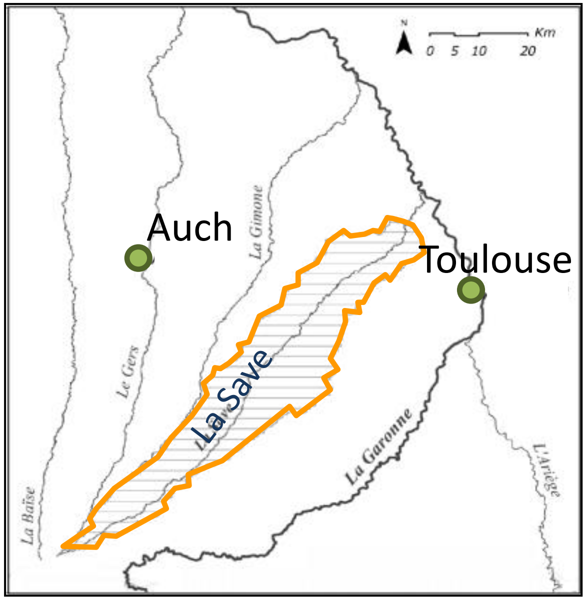
The Save catchment

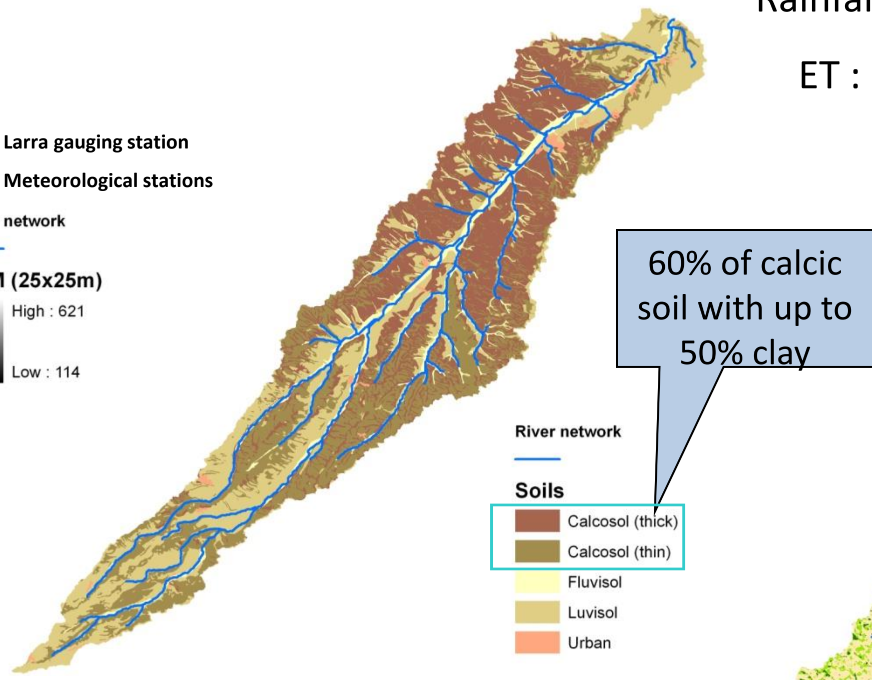
Catchment area : 1117 km²

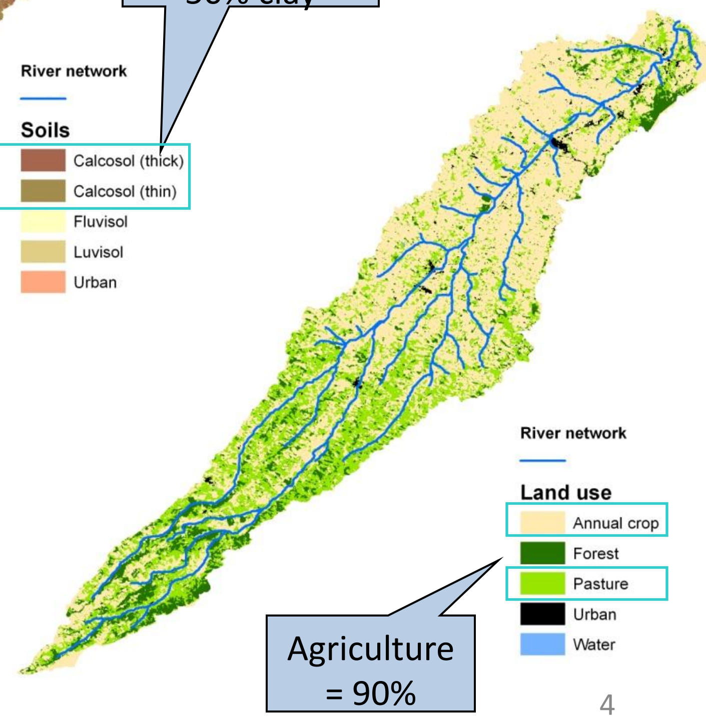
Rainfall : 600-800 mm

ET : 500-600 mm



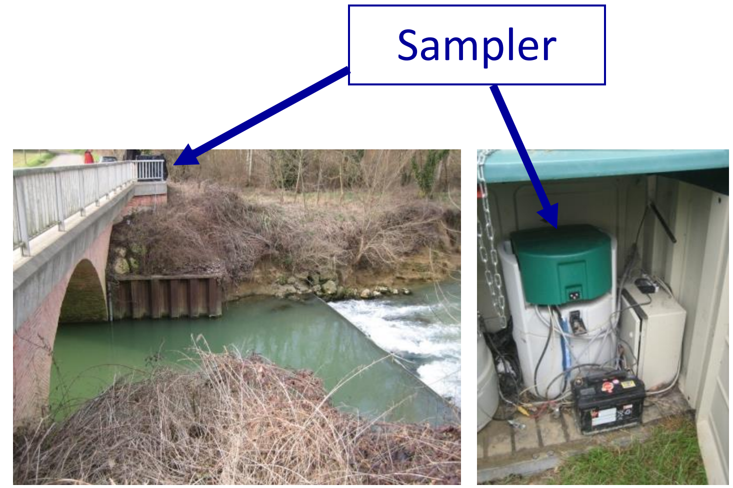


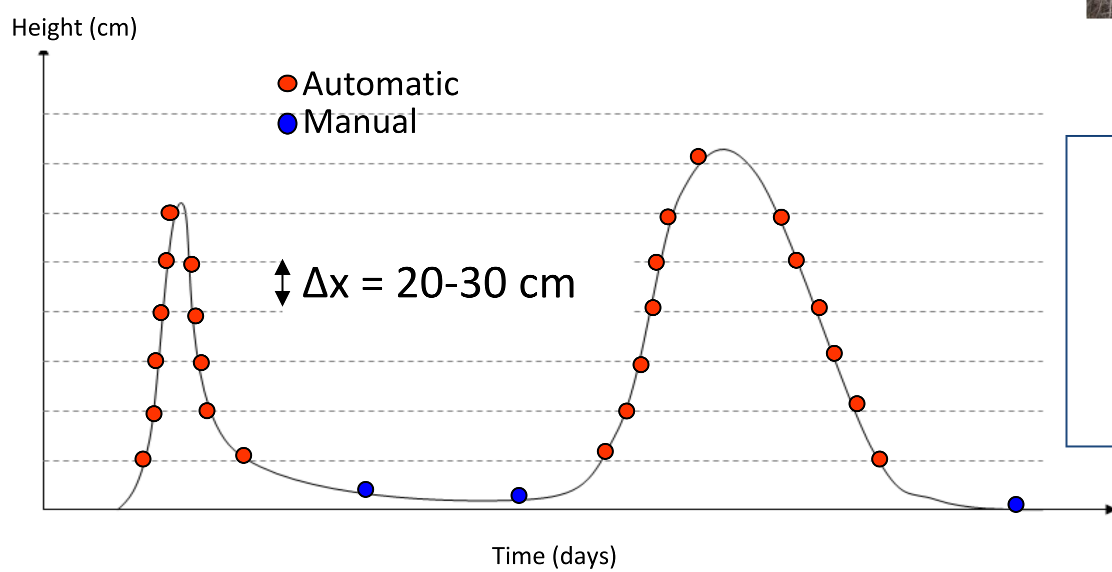




Water quality monitoring

- Hourly discharge
- Particulate Organic Carbon (POC)
- Total suspended matter (TSM)
- Pesticides (dissolved and sorbed)



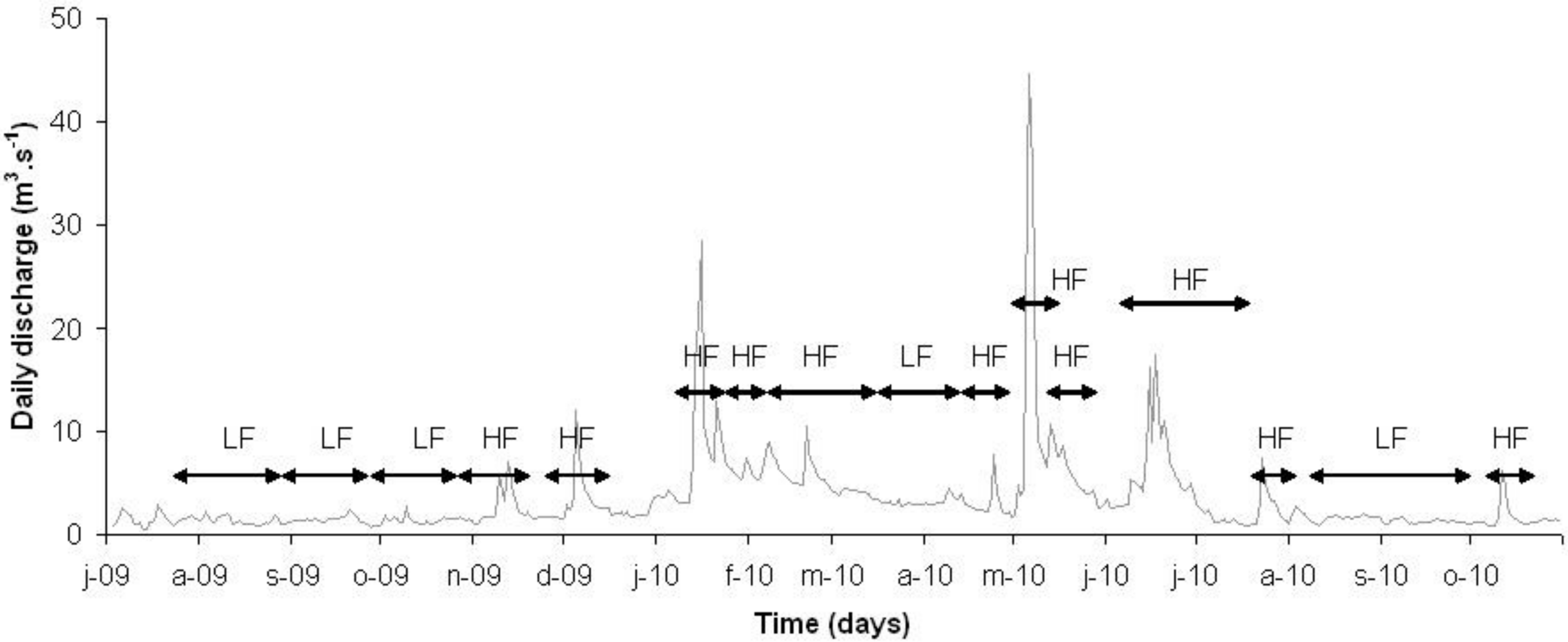


Sampling period = f(water height)

Aguaflash : 242 samples

Laboratory analysis: 46 sought molecules

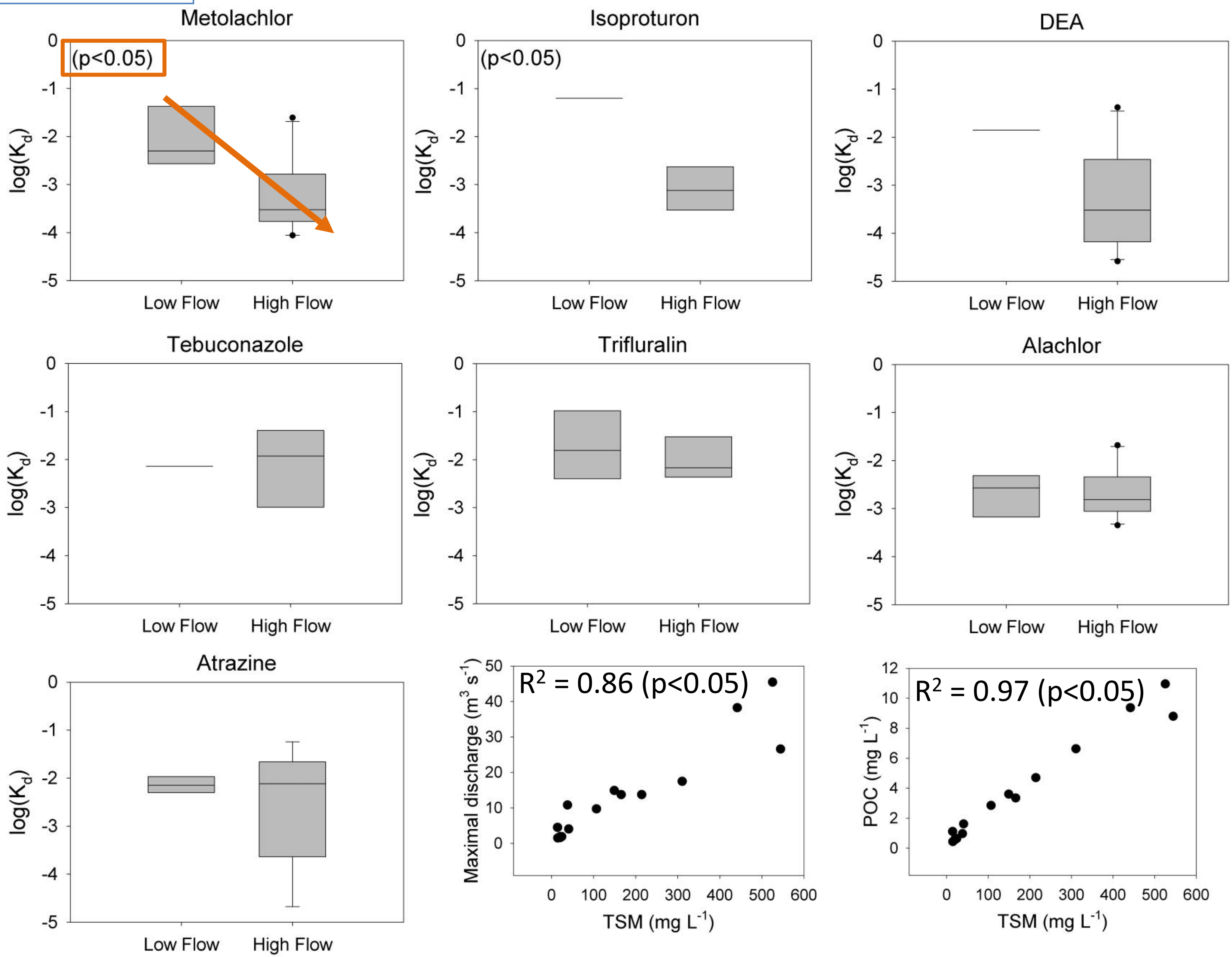
Relationship between Koc and Kow



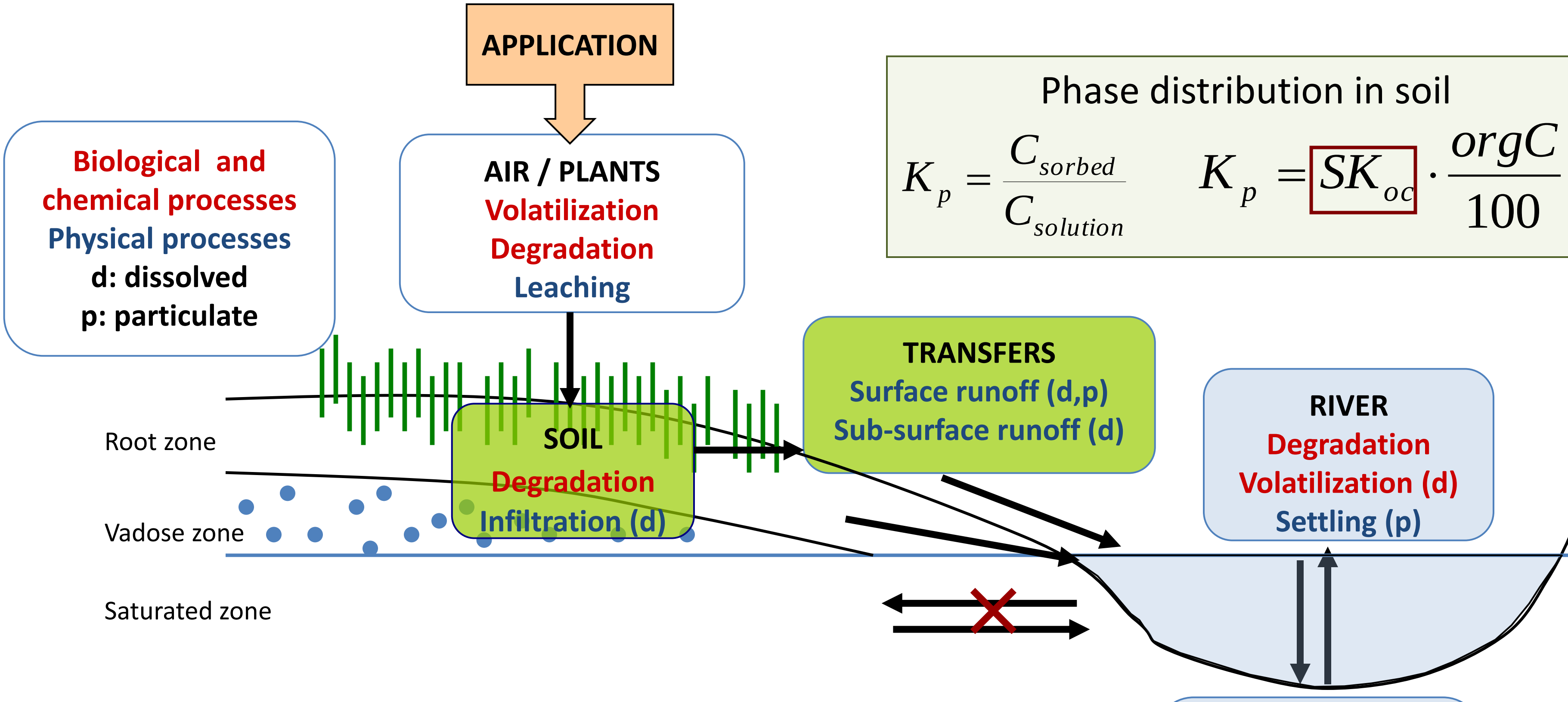
16 hydrological events : 11 high flow periods + 5 low flow periods

Observed pesticide dynamics

$$K_d\left[m^3 g^{-1}\right] = \frac{C_{sorbed}}{C_{soluble}}$$



Pesticide fate modelling with SWAT



Phase distribution in soil

$$K_p = \frac{C_{sorbed}}{C_{solution}} \qquad K_p = \boxed{SK_{oc}} \cdot \frac{orgC}{100}$$

Phase distribution in rivers

$$F_d = \frac{1}{1 + \boxed{CK_{oc}} \cdot conc_{sed}} \qquad F_p = 1 - F_d$$

K_d sensitivity in SWAT

SWAT calibration from Boithias et al.,
In revision, *Region. Environ. Change*

Sentivity analysis : $S_i = \frac{\partial P}{\partial I} \cdot \frac{I}{P(I)}$

S_i mean		Metolachlor	Aclonifen
SK_{oc}	Soil	-0,44	-0,30
CK_{oc}	River	-1,17	-0,95

3x more sensitive

To improve the partition at basin scale -> we focus on Ckoc

From Karickhoff et al. (1979) : $K_d = f_{oc} \cdot K_{oc}$

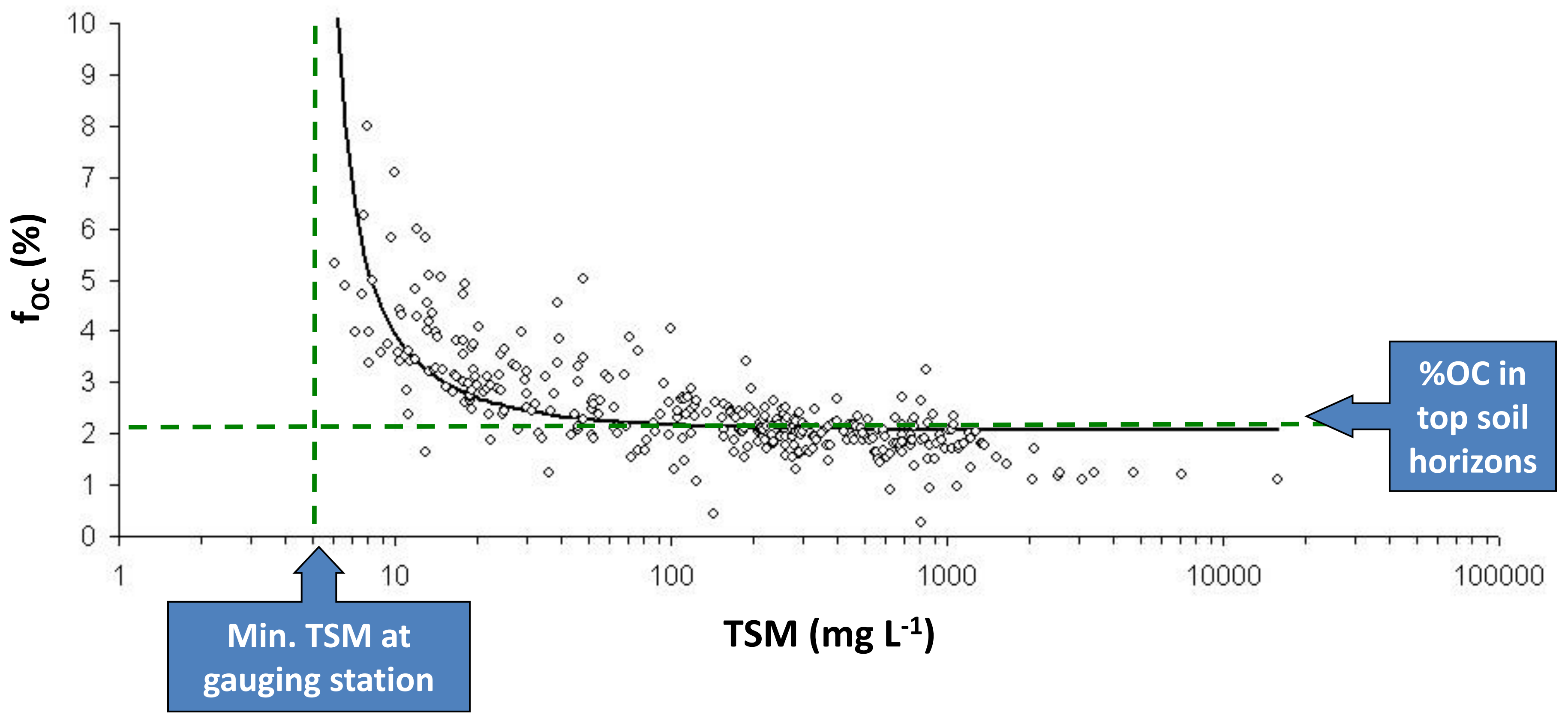
$$K_d = f(TSM) \cdot f(K_{ow})$$

SWAT simulates TSM
K_d is better correlated to TSM than POC

K_{ow} is a standard laboratory value

Relationship between %POC and TSM

Data: 2007-2010 (Aguaflash + Oeurng et al., 2011, *Hydrol. Process.*)



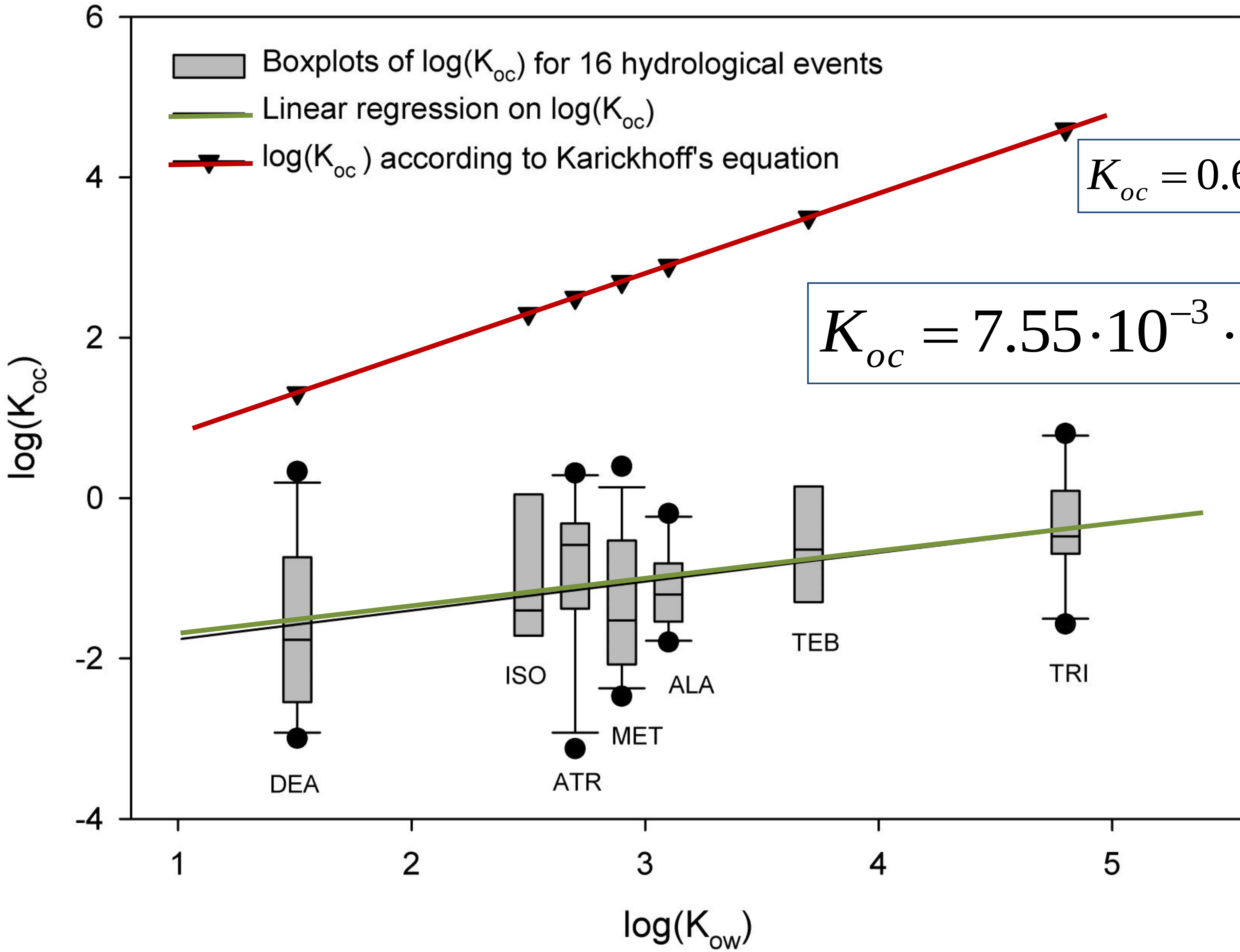
$$f_{oc} = \frac{0.09}{TSM - 5} + 0.02$$

Validity domain: TSM =]5;1000]

When over 1000 mg L^{-1} f_{oc} = 1.6%

$R^2 = 0.6$

Relationship between Koc and Kow

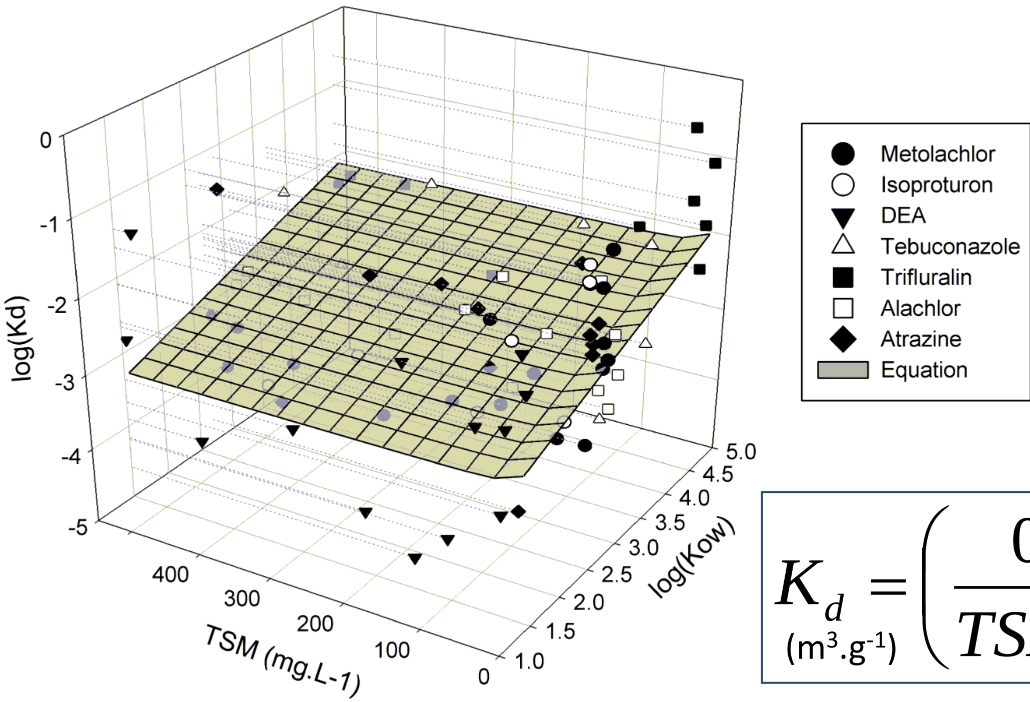


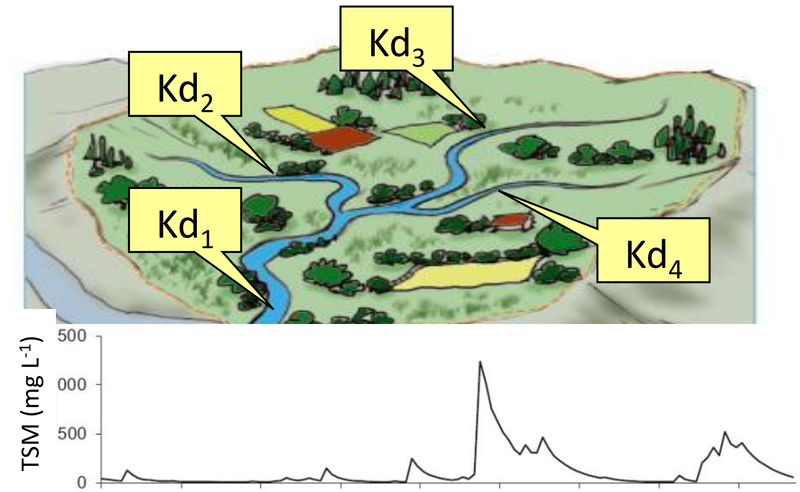
$$K_{oc} = 0.63 \cdot K_{ow}$$

$$K_{oc} = 7.55 \cdot 10^{-3} \cdot K_{ow}^{0.36}$$

$R^2 = 0.8$

Conclusions





$$K_d = \left(\frac{0.09}{TSM - 5} + 0.02 \right) \cdot 7.55 \cdot 10^{-3} \cdot K_{ow}^{0.36}$$

K_d ($m^3.g^{-1}$)

- Method may be applied to a wide range of catchment and organic contaminants
- Equation can be implemented in any model describing the fate of pesticides in both dissolved and sorbed phases
- Currently under revision in Chemosphere

Thanks for your attention !

For further questions :

l.boithias@gmail.com

http://www.aguaflash-sudoe.eu/

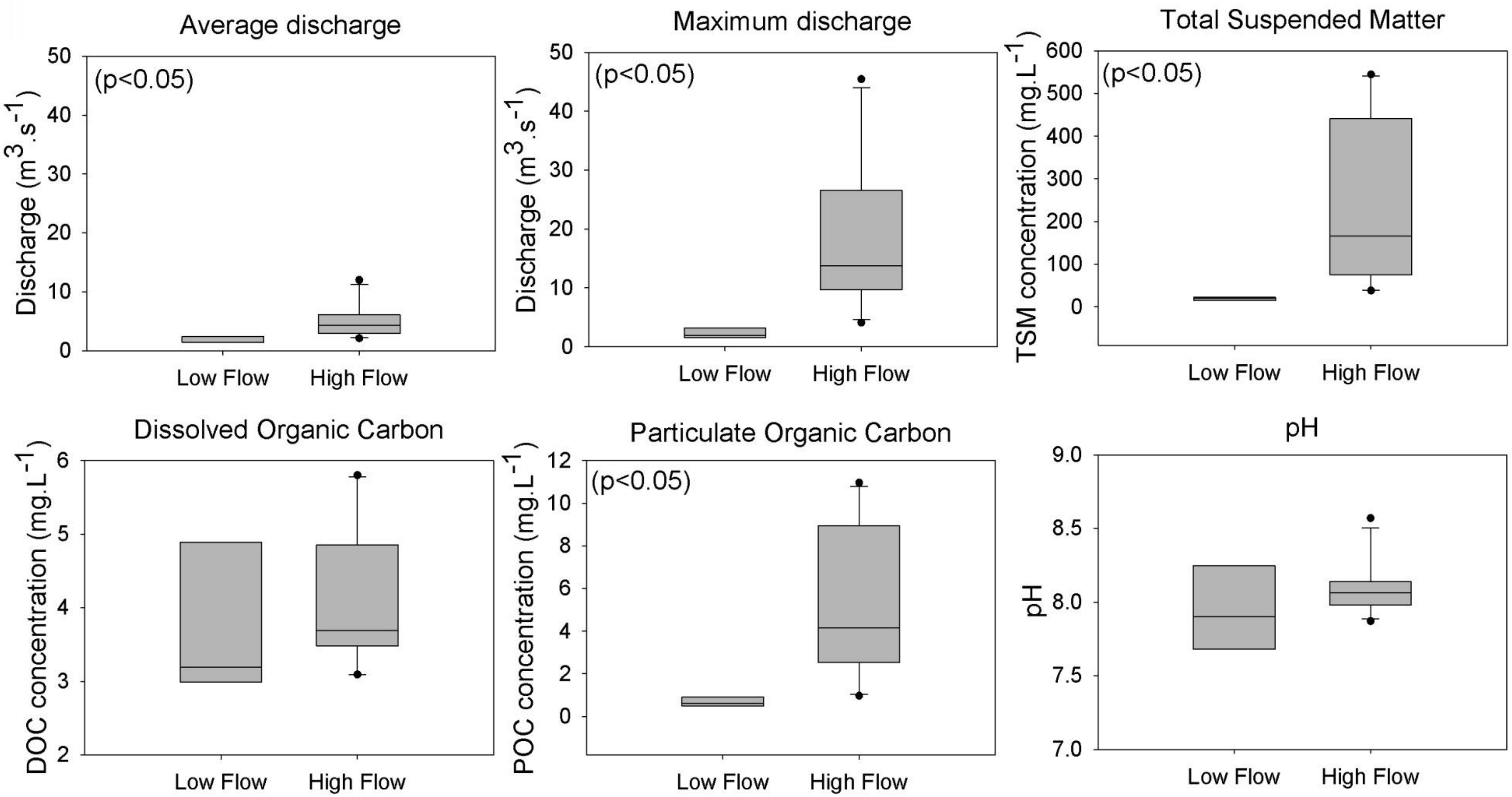
Present address at ICRA, Spain

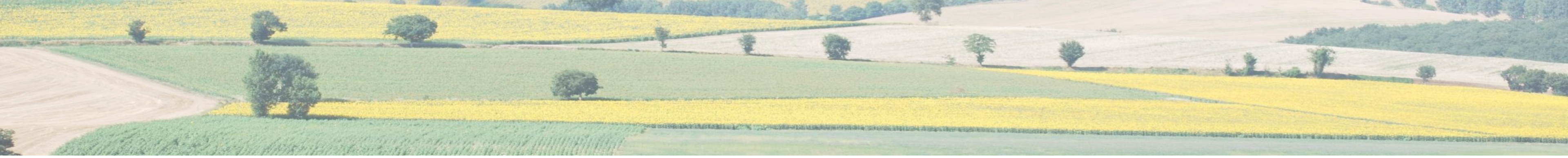
How to aggragte concentrations

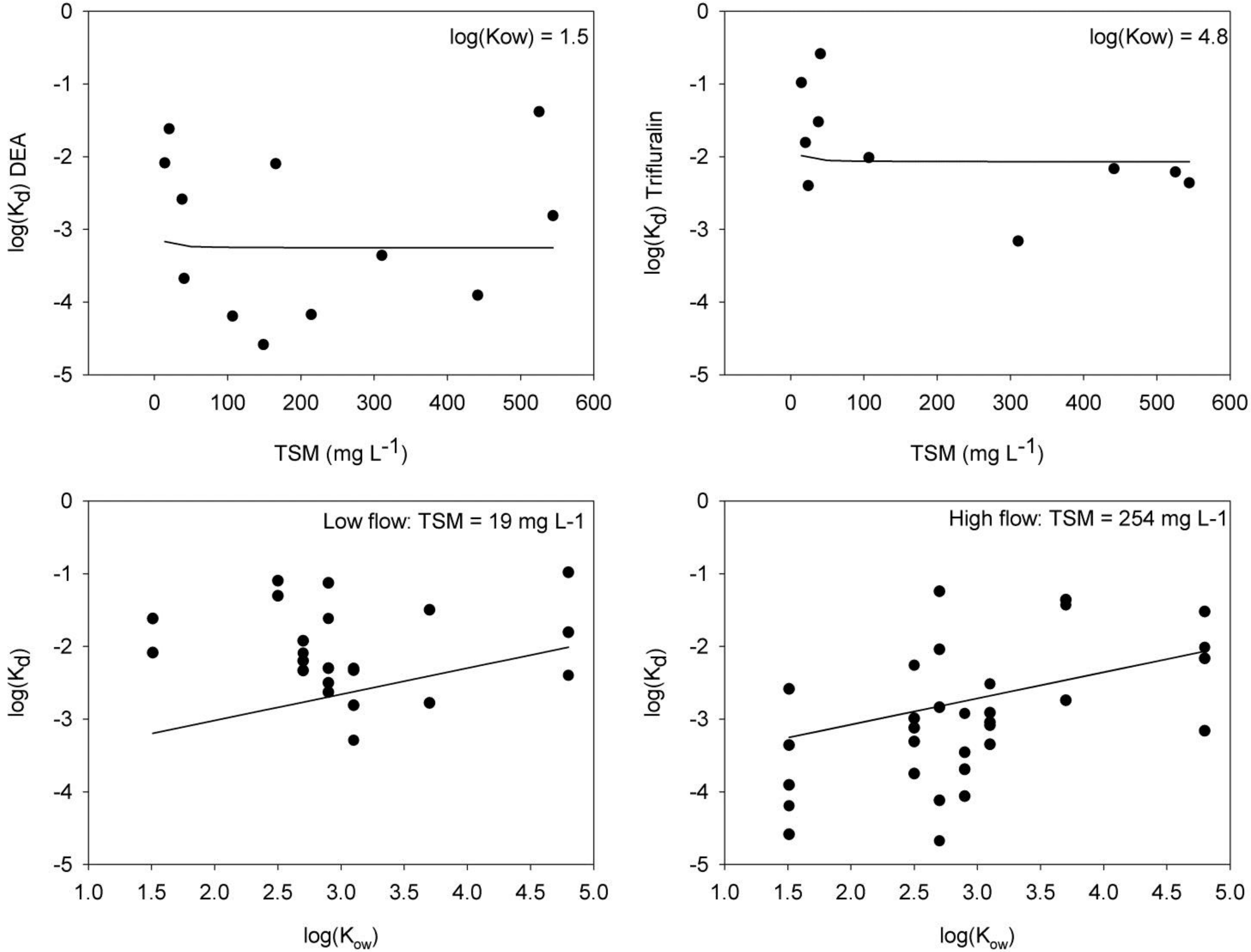
- For each low flow and high flow concentration :

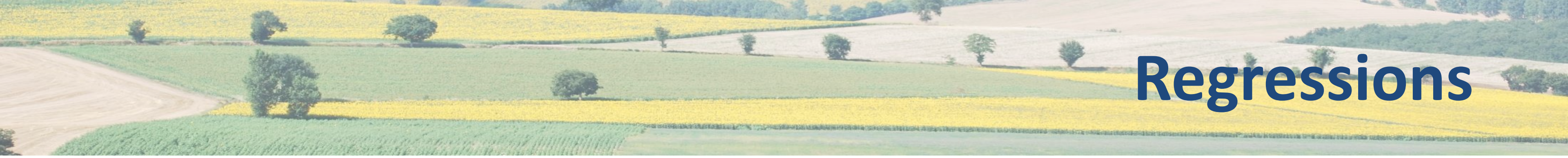
$$C = \frac{C_1 \cdot Q_1 + C_2 \cdot Q_2 + \ldots}{Q_1 + Q_2 + \ldots}$$

Environmental parameters






log(Kow) = 1.5
log(K$_d$) DEA
TSM (mg L^{-1})
log(Kow) = 4.8
log(K$_d$) Trifluralin
TSM (mg L^{-1})
Low flow: TSM = 19 mg L-1
log(K$_d$)
log(K$_{ow}$)
High flow: TSM = 254 mg L-1
log(K$_d$)
log(K$_{ow}$)



Regressions

	TSM		POC		DOC	
	R^2	n	R^2	n	R^2	n
Average Q	0.40 ($p<0.05$)	15	0.48 ($p<0.05$)	15	0.21	14
Maximal Q	0.86 ($p<0.05$)	15	0.92 ($p<0.05$)	15	0.39 ($p<0.05$)	14
pH	0.02	14	0.02	14	0.13	14
POC	0.97 ($p<0.05$)	15	-		-	
DOC	0.39 ($p<0.05$)	14	0.39 ($p<0.05$)	14	-	
K_d alachlor	0.06	14	0.05	14	0.09	13
K_d atrazine	0.04	13	0.05	13	0.04	12
K_d DEA	0.00	12	0.00	12	0.01	12
K_d isoproturon	0.53	7	0.52	7	0.01	7
K_d metolachlor	0.47 ($p<0.05$)	15	0.47 ($p<0.05$)	15	0.16	14
K_d tebuconazole	0.17	7	0.08	7	0.51	6
K_d trifluralin	0.30	10	0.29	10	0.09	9